

=> file registry

FILE 'REGISTRY' ENTERED AT 16:32:07 ON 20 JUL 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 19 JUL 2006 HIGHEST RN 894691-89-5
DICTIONARY FILE UPDATES: 19 JUL 2006 HIGHEST RN 894691-89-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> file hcaplus

FILE 'HCAPLUS' ENTERED AT 16:32:10 ON 20 JUL 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
the American Chemical Society and is provided to assist you in searching
databases on STN. Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 20 Jul 2006 VOL 145 ISS 4
FILE LAST UPDATED: 19 Jul 2006 (20060719/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

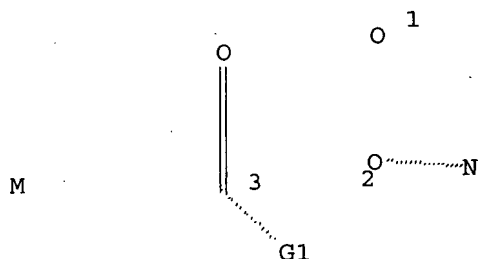
This file contains CAS Registry Numbers for easy and accurate
substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d stat que L74

L40	2034666	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	T1/PG
L41	980214	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	T2/PG
L42	604750	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	T3/PG
L43	2951684	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	(L40 OR L41 OR L42)
L47			STR			

G2



N 4

G1 [@1], [@2]

G2 [@3], [@4]

Structure attributes must be viewed using STN Express query preparation.

```

L49      720204 SEA FILE=REGISTRY ABB=ON  PLU=ON  L43 AND N>2
L51      92776  SEA FILE=REGISTRY SUB=L49 SSS FUL L47
L52      64415  SEA FILE=HCAPLUS ABB=ON  PLU=ON  L51
L53      63198  SEA FILE=HCAPLUS ABB=ON  PLU=ON  "MASS SPECTROMETRY"/CW
L56      145097 SEA FILE=HCAPLUS ABB=ON  PLU=ON  TRANSITION METAL?/OBI
L62      129778 SEA FILE=HCAPLUS ABB=ON  PLU=ON  MASS SPECTROM?/OBI
L63      229730 SEA FILE=HCAPLUS ABB=ON  PLU=ON  MASS SPECTROM?/BI
L66      179531 SEA FILE=HCAPLUS ABB=ON  PLU=ON  TRANSITION METAL?/BI
L72      705    SEA FILE=HCAPLUS ABB=ON  PLU=ON  L52 AND (L53 OR (L62 OR L63))

L73      QUE   ABB=ON  PLU=ON  ?PEPTID?/BI
L74      9     SEA FILE=HCAPLUS ABB=ON  PLU=ON  L73 AND L72 AND (L56 OR L66)

```

=> d ibib abs hitind hitstr L74 1-9

L74 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:564739 HCAPLUS

DOCUMENT NUMBER: 145:58819

TITLE: Labeled **transition metal** complexes
for labeling chemical or biological entities for
mass spectrometry

INVENTOR(S): Lacombe, Marie; Opdam, Franciscus Johannes Marie;
Talman, Eduard Gerhard; Veuskens, Jacky Theo Maria

PATENT ASSIGNEE(S): Kreatech Biotechnology B.V., Neth.

SOURCE: PCT Int. Appl., 91 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006062391	A1	20060615	WO 2005-NL824	20051201
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM EP 1669760 A1 20060614 EP 2004-78328 20041208 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				

PRIORITY APPLN. INFO.: EP 2004-78328 A 20041208

AB The invention relates to a labeled **transition metal** complex comprising a **transition metal** atom, a reactive moiety for allowing a chemical or biol. entity to become attached to the **transition metal** atom, an inert tridentate moiety as a stabilizing bridge, and a marker. The invention also relates to a labeled chemical or biol. entity comprising a chemical or biol. entity which is attached to said labeled **transition metal** complex, to the use of said complex for creating a defined shift in the mol. mass of said entity in order to facilitate **mass spectrometric** anal. of said entity, to methods for rendering chemical or biol. entities distinguishable by **mass spectrometry** as well as to methods for **mass spectrometric** anal. of the chemical or biol. entities. In addition, the present invention also relates to a set of at least two of said **transition metal** complexes of different mol. mass, to **transition metal** complexes comprising different stable isotopes, to chemical or biol. entities obtained by a method of the invention and to a kit of parts supporting the use and/or methods of the invention. 4'-Aminopentyl ether-2,2':6',2"-terpyridine (APET), prepared from 5-aminopentanol and 4'-chloro-2,2':6',2"-terpyridine, was coupled with EZ-link-LC-biotin succinimidyl ester and complexed with K₂PtCl₄. The complex was used to label proteins and DNA.

CC 9-5 (Biochemical Methods)

Section cross-reference(s): 28, 29, 78

ST labeled **transition metal** complex labeling **mass spectrometry**; biotin aminopentyl ether terpyridine platinum complex labeling protein; DNA labeling biotin aminopentyl ether terpyridine platinum complex

IT Nucleic acid hybridization
 (DNA-DNA, in situ; labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT Antibodies and Immunoglobulins

RL: RCT (Reactant); RACT (Reactant or reagent)
 (IgA, labeling of; labeled **transition metal**)

- complexes for labeling chemical or biol. entities for **mass spectrometry**)
- IT Antibodies and Immunoglobulins
RL: RCT (Reactant); RACT (Reactant or reagent)
(IgG; labeling of; labeled **transition metal**
complexes for labeling chemical or biol. entities for **mass spectrometry**)
- IT Antibodies and Immunoglobulins
RL: RCT (Reactant); RACT (Reactant or reagent)
(IgM; labeling of; labeled **transition metal**
complexes for labeling chemical or biol. entities for **mass spectrometry**)
- IT Ionic strength
(agents for adjustment of; labeled **transition metal**
complexes for labeling chemical or biol. entities for **mass spectrometry**)
- IT Glycosides
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(amino, aminoglycosides, labeled with labeled **transition metal** complex; labeled **transition metal**
complexes for labeling chemical or biol. entities for **mass spectrometry**)
- IT Samples
(anal. of; labeled **transition metal** complexes for
labeling chemical or biol. entities for **mass spectrometry**)
- IT Phosphate group
(as reactive group in labeled **transition metal**
complex; labeled **transition metal** complexes for
labeling chemical or biol. entities for **mass spectrometry**)
- IT Bicarbonates
Bromides, reactions
Carbonates, reactions
Chlorides, reactions
Fluorides, reactions
Iodides, reactions
Nitrates, reactions
Phosphonates
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(as reactive group in labeled **transition metal**
complex; labeled **transition metal** complexes for
labeling chemical or biol. entities for **mass spectrometry**)
- IT Immunoassay
(enzyme-linked immunosorbent assay; labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)
- IT Immunoassay
(immunoblotting; labeled **transition metal** complexes
for labeling chemical or biol. entities for **mass spectrometry**)
- IT Fluorescent substances
(in labeled **transition metal** complex; labeled
transition metal complexes for labeling chemical or
biol. entities for **mass spectrometry**)
- IT Buffers
Human

Mass spectrometry
Microarray technology
Tandem mass spectrometry
Test kits
Test tubes
 (labeled **transition metal** complexes for labeling
 chemical or biol. entities for **mass spectrometry**)
IT Polyoxyalkylenes, reactions
 Transition metals, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (labeled **transition metal** complexes for labeling
 chemical or biol. entities for **mass spectrometry**)
IT Amines, biological studies
Amino acids, biological studies
Enzymes, biological studies
Glycoproteins
Nucleosides, biological studies
 Oligopeptides
 Peptide nucleic acids
Phospholipids, biological studies
Polynucleotides
 RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic
 preparation); BIOL (Biological study); PREP (Preparation)
 (labeled with labeled **transition metal** complex;
 labeled **transition metal** complexes for labeling
 chemical or biol. entities for **mass spectrometry**)
IT Antibodies and Immunoglobulins
Nucleic acids
Nucleotides, biological studies
Oligonucleotides
 Peptides, biological studies
Proteins
 RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic
 preparation); BIOL (Biological study); PREP (Preparation)
 (labeled, with labeled **transition metal** complex;
 labeled **transition metal** complexes for labeling
 chemical or biol. entities for **mass spectrometry**)
IT **Transition metal** complexes
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (labeled; labeled **transition metal** complexes for
 labeling chemical or biol. entities for **mass**
 spectrometry)
IT Plasmids
 (labeling DNA of; labeled **transition metal**
 complexes for labeling chemical or biol. entities for **mass**
 spectrometry)
IT Biochemical compounds
Chemical compounds
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
 (labeling and **mass spectrometry** of; labeled
 transition metal complexes for labeling chemical or
 biol. entities for **mass spectrometry**)
IT HeLa cell
 (labeling lysate proteins of; labeled **transition**
 metal complexes for labeling chemical or biol. entities for
 mass spectrometry)
IT DNA
Proteins
RNA

- RL: RCT (Reactant); RACT (Reactant or reagent)
(labeling of; labeled **transition metal** complexes
for labeling chemical or biol. entities for **mass
spectrometry**)
- IT Mass
(sulfate; labeled **transition metal** complexes for
labeling chemical or biol. entities for **mass
spectrometry**)
- IT Isotopes
RL: PRP (Properties)
(of **transition metal**, complexes containing; labeled
transition metal complexes for labeling chemical or
biol. entities for **mass spectrometry**)
- IT Carboxylic acids, reactions
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(salts, as reactive group in labeled **transition metal**
complex; labeled **transition metal** complexes for
labeling chemical or biol. entities for **mass
spectrometry**)
- IT Functional groups
(sulfate, as reactive group in labeled **transition
metal** complex; labeled **transition metal**
complexes for labeling chemical or biol. entities for **mass
spectrometry**)
- IT Enzymes, biological studies
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic
preparation); BIOL (Biological study); PREP (Preparation)
(synthetic, labeled with labeled **transition metal**
complex; labeled **transition metal** complexes for
labeling chemical or biol. entities for **mass
spectrometry**)
- IT Analytical apparatus
(test strips; labeled **transition metal** complexes
for labeling chemical or biol. entities for **mass
spectrometry**)
- IT 146368-14-1D, Cy5, conjugate with APET, platinum and ruthenium
146368-16-3D, Cy3, conjugate with APET-Pt 890935-62-3D,
conjugate with Cy5 890935-70-3D, conjugate with Cy3 and Cy5
RL: RCT (Reactant); RACT (Reactant or reagent)
(DNA labeling with; labeled **transition metal**
complexes for labeling chemical or biol. entities for **mass
spectrometry**)
- IT 64-19-7, Acetic acid, reactions 71-50-1, Acetate, reactions 77-92-9,
reactions 126-44-3, Citrate, reactions 144-62-7, Ethanedioic acid,
reactions 338-70-5, reactions 625-58-1, Ethylnitrate 7732-18-5,
Water, reactions
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(as reactive group in labeled **transition metal**
complex; labeled **transition metal** complexes for
labeling chemical or biol. entities for **mass
spectrometry**)
- IT 111-40-0, Diethylenetriamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation of; labeled **transition metal**
complexes for labeling chemical or biol. entities for **mass
spectrometry**)
- IT 890935-60-1 890935-61-2
RL: ARG (Analytical reagent use); PRP (Properties); RCT (Reactant); ANST
(Analytical study); RACT (Reactant or reagent); USES (Uses)

(labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT 890935-50-9P
 RL: ARG (Analytical reagent use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT 890935-52-1 890935-53-2 890935-54-3 890935-55-4 890935-56-5
 890935-57-6 890935-58-7 890935-59-8
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
 (labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT 890935-49-6P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT 79-04-9, Chloroacetyl chloride 107-13-1, Acrylonitrile, reactions
 107-14-2, Chloroacetonitrile, 107-15-3, Ethylenediamine, reactions
 627-42-9, 2-Chloroethyl methyl ether 1001-53-2, N-Acetyethylenediamine
 2508-29-4, 5-Aminopentanol 7439-88-5D, Iridium, complexes 7439-89-6D,
 Iron, complexes 7439-96-5D, Manganese, complexes 7439-98-7D,
 Molybdenum, complexes 7440-02-0D, Nickel, complexes 7440-04-2D,
 Osmium, complexes 7440-05-3D, Palladium, complexes 7440-06-4D,
 Platinum, complexes 7440-16-6D, Rhodium, complexes 7440-18-8D,
 Ruthenium, complexes 7440-33-7D, Tungsten, complexes 7440-43-9D,
 Cadmium, complexes 7440-47-3D, Chromium, complexes 7440-48-4D, Cobalt,
 complexes 7440-50-8D, Copper, complexes 7440-62-2D, Vanadium,
 complexes 7440-66-6D, Zinc, complexes 10025-99-7 25322-68-3,
 Polyethylene glycol 51857-17-1 62572-85-4 72040-63-2 92557-81-8
 128143-89-5 139346-57-9 150810-69-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

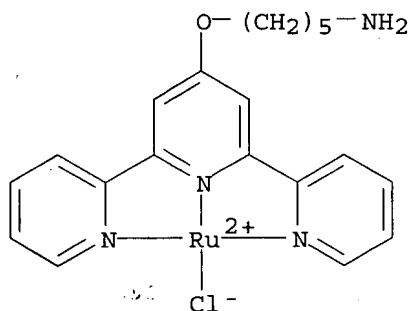
IT 111-40-ODP, Diethylenetriamine, complex with platinum compds.
 86240-79-1P 194213-77-9P 201282-04-4P 672304-28-8P 869484-26-4P
 890648-50-7P 890648-51-8P 890648-55-2P 890648-56-3P 890648-57-4P
 890648-58-5P 890648-59-6P 890648-60-9P 890648-61-0P 890935-47-4P
 890935-48-5P 890935-65-6P 890935-66-7P 890935-68-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT 890648-52-9P 890648-53-0P 890648-54-1P 890935-69-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

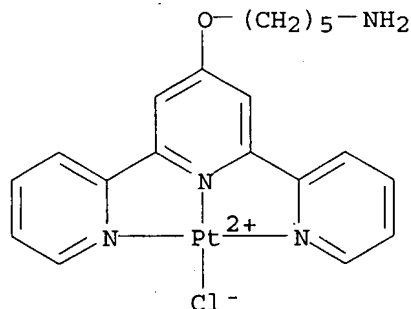
IT 75909-25-0
 RL: BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
 (labeling of; labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT 890935-63-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and HeLa cell lysate protein labeling with; labeled **transition metal** complexes for labeling chemical or

- biol. entities for **mass spectrometry**)
- IT 890935-64-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and plasmid DNA labeling with; labeled **transition
 metal complexes for labeling chemical or biol. entities for
 mass spectrometry**)
- IT 890935-67-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and protein labeling with; labeled **transition
 metal complexes for labeling chemical or biol. entities for
 mass spectrometry**)
- IT 890935-51-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction with DNA; labeled **transition metal
 complexes for labeling chemical or biol. entities for mass
 spectrometry**)
- IT 890935-62-3D, conjugate with Cy5, 890935-70-3D, conjugate
 with Cy3 and Cy5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (DNA labeling with; labeled **transition metal
 complexes for labeling chemical or biol. entities for mass
 spectrometry**)
- RN 890935-62-3 HCAPLUS
 CN INDEX NAME NOT YET ASSIGNED



RN 890935-70-3 HCAPLUS
 CN INDEX NAME NOT YET ASSIGNED



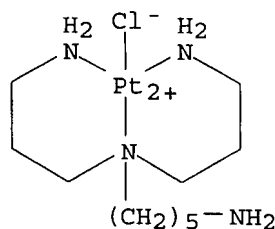
IT 890935-48-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(labeled **transition metal** complexes for labeling
chemical or biol. entities for **mass spectrometry**)

RN 890935-48-5 HCAPLUS

CN INDEX NAME NOT YET ASSIGNED



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L74 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1354663 HCAPLUS

DOCUMENT NUMBER: 144:83644

TITLE: Methods for target molecule detection using
siderophores and related compositions

INVENTOR(S): Bosse, Roger; Patton, Wayne F.; Roby, Philippe

PATENT ASSIGNEE(S): PerkinElmer Las, Inc., USA

SOURCE: PCT Int. Appl., 47 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005123954	A2	20051229	WO 2005-US20152	20050609
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

US 2006019279 A1 20060126 US 2005-148478 20050609

PRIORITY APPLN. INFO.: US 2004-521644P P 20040609

US 2004-521956P P 20040727

AB The invention provides methods for isolating a target mol. from a sample.
In an embodiment, the method involves contacting a sample with a capture
agent, the agent comprising a siderophore and a **transition**
metal cation, under conditions wherein the agent is capable of
binding a target mol. to form a target mol.-capture agent complex, wherein
the target mol. is selected from the group consisting of a phosphorylated

mol., a nitrotyrosine-containing mol. and a sulfated mol., and separating the target mol.-capture agent complex from the sample, thereby isolating the target mol. from the sample. Also provided are methods for determining the presence of a target mol. in a sample, that involve contacting a sample with a capture agent, the agent comprising a siderophore and a transition metal ion.

IC ICM C12Q001-68

CC 9-15 (Biochemical Methods)

IT **Peptides**, uses

RL: NUU (Other use, unclassified); USES (Uses)

(Amphibactins; methods for target mol. detection using siderophores and related compns.)

IT **Peptides**, uses

RL: NUU (Other use, unclassified); USES (Uses)

(Aquachelins; methods for target mol. detection using siderophores and related compns.)

IT **Peptides**, uses

RL: NUU (Other use, unclassified); USES (Uses)

(Marinobactins; methods for target mol. detection using siderophores and related compns.)

IT **Peptides**, uses

RL: NUU (Other use, unclassified); USES (Uses)

(exochelins; methods for target mol. detection using siderophores and related compns.)

IT **Transition metals**, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(ions; methods for target mol. detection using siderophores and related compns.)

IT Absorption

Atomic spectrometry

Capillary tubes

Composition

ESR (electron spin resonance)

Ellipsometry

Filters

Gels

Mass

Mass spectrometry

Matrix media

Membranes, nonbiological

Microarray technology

NMR (nuclear magnetic resonance)

Particles

Phosphorylation, biological

Polarized fluorescence

Refractive index

Resonance fluorescence

SERS (Raman scattering)

Surface

Surface plasmon resonance

Transmissions (mechanical)

(methods for target mol. detection using siderophores and related compns.)

IT **Peptides**, uses

RL: NUU (Other use, unclassified); USES (Uses)

(methods for target mol. detection using siderophores and related compns.)

IT **Peptides**, uses

RL: NUU (Other use, unclassified); USES (Uses)

(ornibactins; methods for target mol. detection using siderophores and related compns.)

IT **Mass spectrometry**

(plasma-source, inductively-coupled; methods for target mol. detection using siderophores and related compns.)

IT 51-28-5, 2,4-Dinitrophenol, uses 58-85-5, Biotin 94-75-7, 2,4-Dichlorophenoxyacetic acid, uses 533-48-2, Desthiobiotin 1400-46-0, Mycobactin 1672-46-4, Digoxigenin 2396-01-2, Phenyl 8062-00-8, Pyoverdin 9001-45-0 9003-99-0, Peroxidase 9031-11-2, β -Galactosidase 11115-85-8, Fusarinine **12705-44-1**, Coprogen B **12705-44-1D**, Coprogen B, derivs. 15646-46-5 15788-16-6, 5-Benzimidazolecarboxylic acid 18928-00-2, Rhodotorulic acid 23086-46-6, Ferricrocin 23425-25-4, Ferrirubin 26912-16-3D, Dimerum acid, derivs. 28384-96-5, Enterobactin 35418-52-1, Schizokinen 72731-33-0, Cepabactin 79236-62-7 104022-79-9, Pyoverdin Pa A 114844-84-7, Azotobactin 120124-51-8, Chrysobactin 124620-50-4, EKD 3-88 131688-65-8, Azoverdin 134782-23-3, JAM-2-263 139917-13-8, Pseudobactin B 10 156737-07-4, Acinetoferrin 159074-16-5, Alcaligin E 197846-90-5, Pyoverdin G4R 207130-71-0D, Vicibactin, derivs. 214491-43-7, 6,8-Difluoro-4-methylumbelliferyl phosphate 344549-56-0 353512-65-9, Triacetylfusarinine

RL: NUU (Other use, unclassified); USES (Uses)

(methods for target mol. detection using siderophores and related compns.)

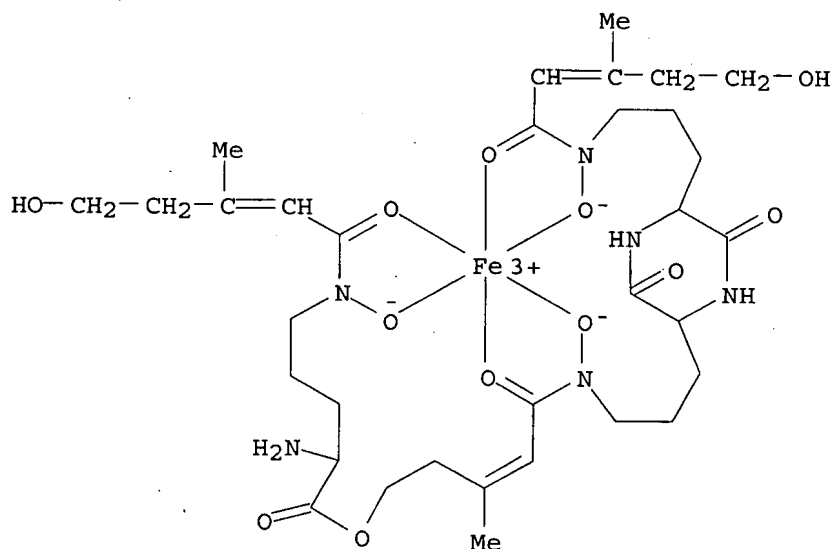
IT **12705-44-1**, Coprogen B **12705-44-1D**, Coprogen B, derivs.

RL: NUU (Other use, unclassified); USES (Uses)

(methods for target mol. detection using siderophores and related compns.)

RN **12705-44-1** HCAPLUS

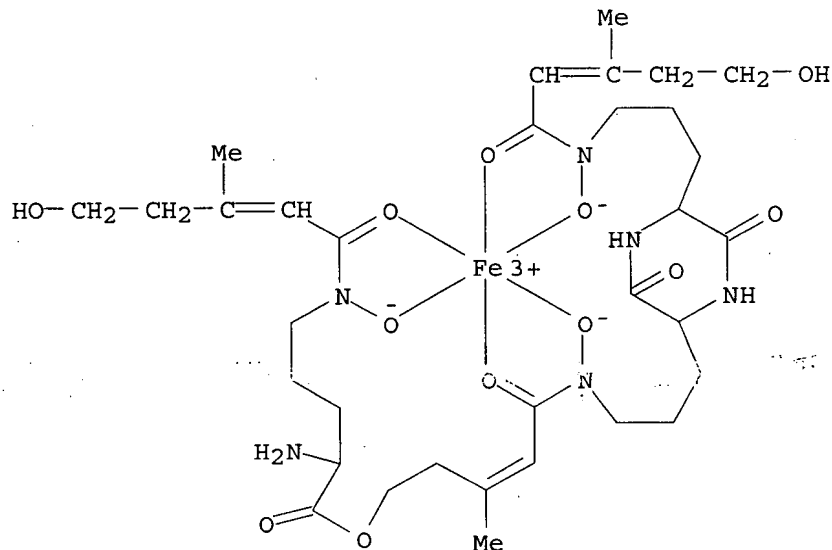
CN Iron, [5-[(hydroxy- κ O) [3-[5-[3-[(hydroxy- κ O) [5-hydroxy-3-methyl-1-(oxo- κ O)-2-pentenyl]amino]propyl]-3,6-dioxo-2-piperazinyl]propyl]amino]-3-methyl-5-(oxo- κ O)-3-pentenyl N5-(hydroxy- κ O)-N5-[5-hydroxy-3-methyl-1-(oxo- κ O)-2-pentenyl]-L-ornithinato(3-)]- (9CI) (CA INDEX NAME)



RN **12705-44-1** HCAPLUS

CN Iron, [5-[(hydroxy- κ O) [3-[5-[3-[(hydroxy- κ O) [5-hydroxy-3-

methyl-1-(oxo-κO)-2-pentenyl]amino]propyl]-3,6-dioxo-2-piperazinyl]propyl]amino]-3-methyl-5-(oxo-κO)-3-pentenyl N5-(hydroxy-κO)-N5-[5-hydroxy-3-methyl-1-(oxo-κO)-2-pentenyl]-L-ornithinato(3-)]- (9CI) (CA INDEX NAME)



L74 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1028896 HCAPLUS

DOCUMENT NUMBER: 143:471915

TITLE: Pyridine-Substituted **oligopeptides** as Scaffolds for the Assembly of Multimetallic Complexes: Variation of Chain Length

AUTHOR(S): Ohr, Kristi; Gilmartin, Brian P.; Williams, Mary Elizabeth

CORPORATE SOURCE: Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA

SOURCE: Inorganic Chemistry (2005), 44(22), 7876-7885
CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This paper presents the synthesis and characterization of pyridine-substituted artificial **oligopeptides** with an aminoethylglycine backbone of varying length, which are designed to act as scaffolds for the self-assembly of multimetallic structures. The identities and purities of the **oligopeptides** are confirmed with **mass spectrometry**, ¹H NMR, HPLC, and pH titrns. The acid dissociation consts. for the **oligopeptides** were determined and were found to decrease with increasing pyridine units. Titrns. of the **oligopeptides** with Cu(II) and Pt(II) complexes containing the tridentate ligands 2,2':6',2''-terpyridine and pyridine 2,6-dicarboxylic acid were monitored using UV-visible absorption spectroscopy and showed stoichiometric binding based on the number of pyridines on the **peptide** strand. Metal titrns. performed using an analogous **oligopeptide** with Me substituents (in place of the pyridine ligands) showed very weak or no binding. In the case of the **oligopeptides** containing bound Pt(terpyridine)₂²⁺ complexes, cyclic

- voltammetry reveals two sequential 1-electron redns. at formal potentials that do not vary as a function of **oligopeptide** length. The measured diffusion coeffs. were measured with chronoamperometry and were found to decrease with increasing **oligopeptide** length.
- CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 34, 68, 72
- ST **oligopeptide** pyridyl prepn acidity coordination
transition metal chelate; copper complex pyridyl
oligopeptide scaffold prepn; platinum complex pyridyl
oligopeptide scaffold prepn electrochem redox
- IT Ionization constant
(acidity constant; of pyridine-substituted **oligopeptides**)
- IT Redox reaction
(electrochem.; of pyridine-substituted **oligopeptide** scaffolds coordinated with copper(II) or platinum(II) chelates)
- IT Chemical chains
(length; preparation of pyridine-substituted **oligopeptide** scaffolds, acid dissociation consts., and coordination with copper(II) or platinum(II) chelates)
- IT Formal potential
Reduction potential
Self-assembly
(of pyridine-substituted **oligopeptide** scaffolds coordinated with copper(II) or platinum(II) chelates)
- IT **Oligopeptides**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyridine-substituted **oligopeptide** scaffolds, acid dissociation consts., and coordination with copper(II) or platinum(II) chelates)
- IT 169396-89-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-acylation for preparation of pyridine-substituted **oligopeptide** scaffolds coordinated with metal(II) chelates)
- IT 869190-58-9 869190-60-3 869190-62-5
869190-64-7 869289-03-2
RL: PRP (Properties)
(energy-minimized mol. structure from mol. mechanics calcns.)
- IT 6622-91-9, 4-Pyridylacetic acid hydrochloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of pyridine-substituted **oligopeptide** scaffolds coordinated with metal(II) chelates)
- IT 869190-67-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of pyridine-substituted **oligopeptide** scaffolds coordinated with metal(II) chelates)
- IT 220802-14-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of tetramer **oligopeptide** scaffold)
- IT 861886-02-4P 861886-04-6P 869190-49-8P
869190-50-1P 869190-51-2P 869190-53-4P
869190-55-6P 869190-57-8P 869287-59-2P 869288-33-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyridine-substituted **oligopeptide** scaffolds coordinated with metal(II) chelates)
- IT 869190-59-0P 869190-61-4P 869190-63-6P
869190-65-8P 869289-23-6P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation, cyclic voltammetry, and diffusion coefficient measured with chronoamperometry)

IT 869190-64-7

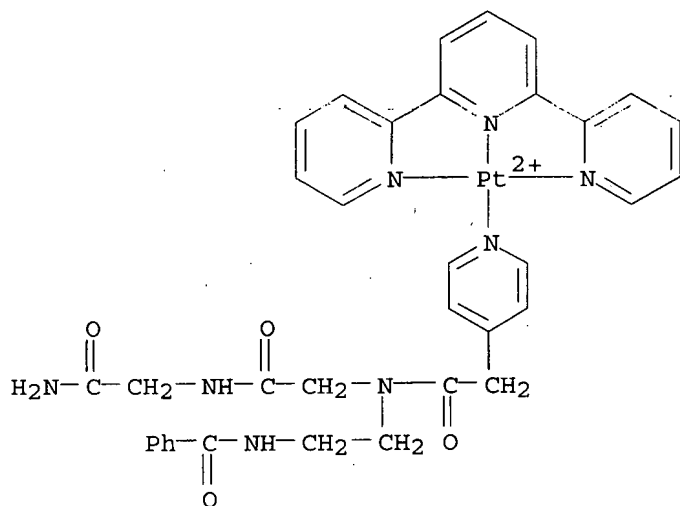
869190-64-7

RL: PRP (Properties)

(energy-minimized mol. structure from mol. mechanics calcns.)

RN 869190-58-9 HCAPLUS

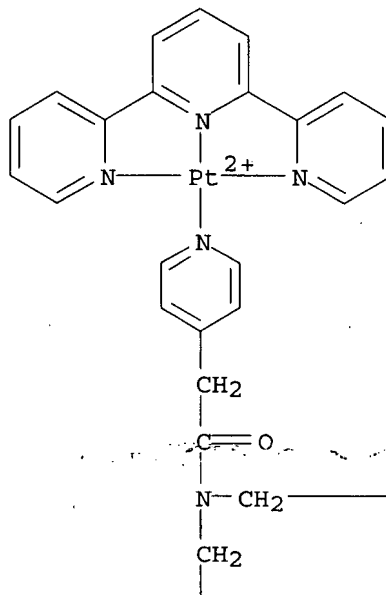
CN Platinum(2+), [N-[2-(benzoylamino)ethyl]-N-[(4-pyridinyl- κ N)acetyl]glycylglycinamide] (2,2':6',2''-terpyridine- κ N1, κ N1', κ N1'')-, (SP-4-3)- (9CI) (CA INDEX NAME)



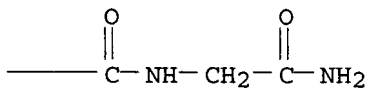
RN 869190-60-3 HCAPLUS

CN Platinum(8+), [μ 4-[N-[(4-pyridinyl- κ N)acetyl]-N-[4,10,16,22-tetraoxo-22-phenyl-6,12,18-tris[(4-pyridinyl- κ N)acetyl]-3,6,9,12,15,18,21-heptaazadocos-1-yl]glycylglycinamide]]tetrakis(2,2':6',2''-terpyridine- κ N1, κ N1', κ N1'')tetra- (9CI) (CA INDEX NAME)

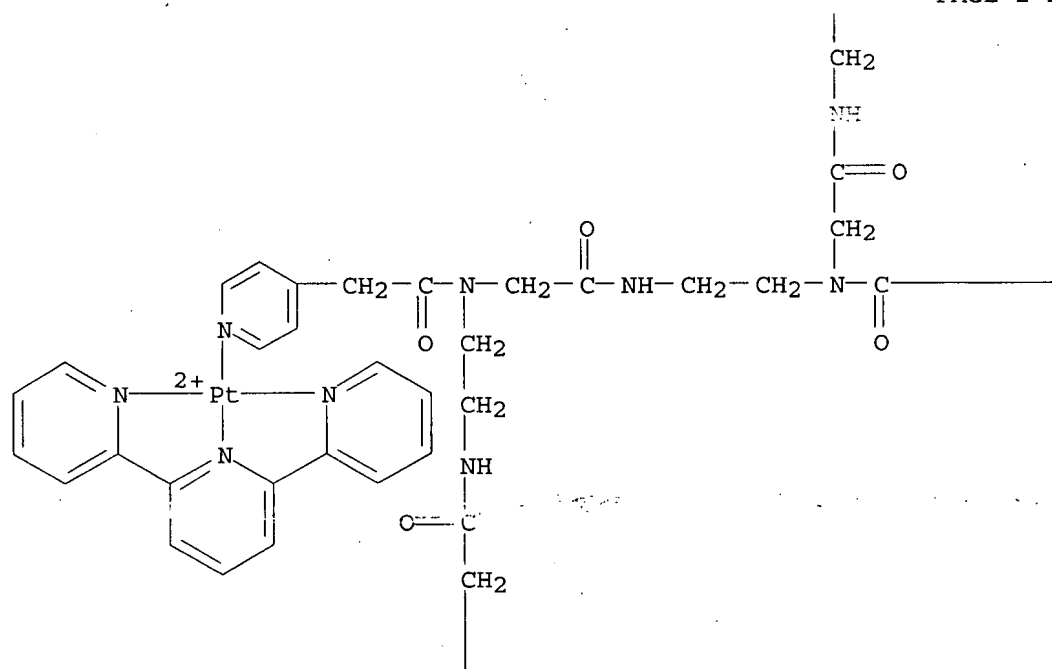
PAGE 1-A



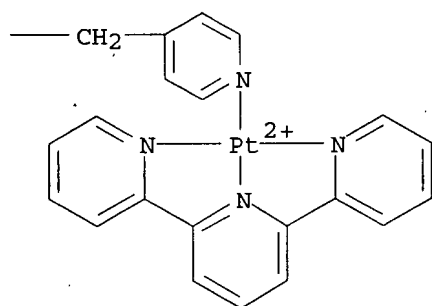
PAGE 1-B



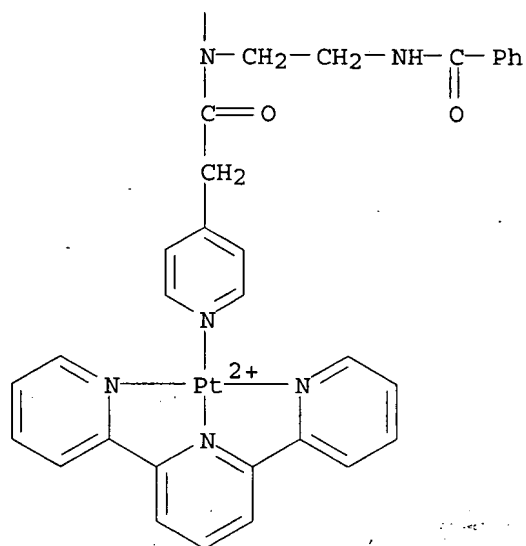
PAGE 2-A



PAGE 2-B

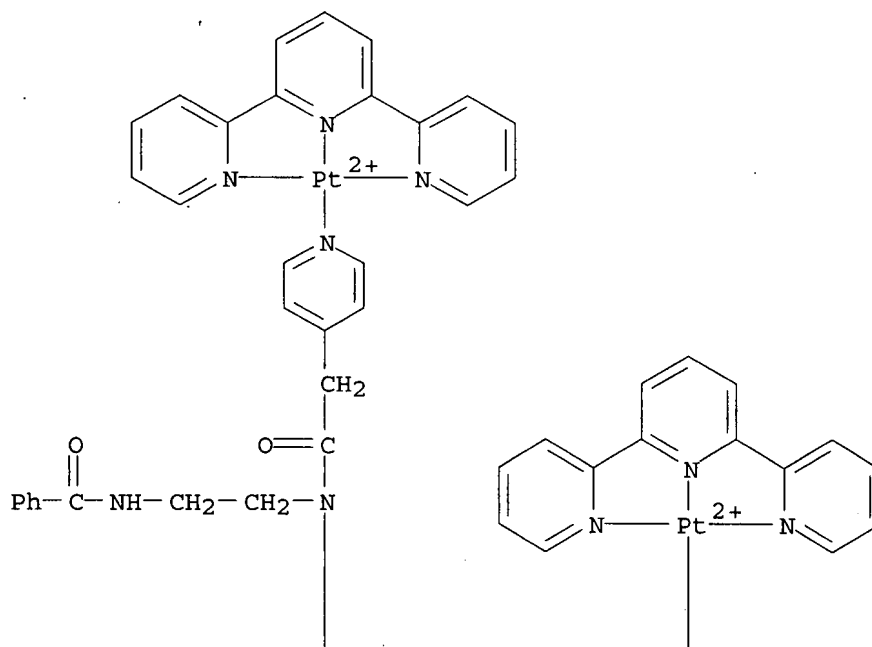


PAGE 3-A

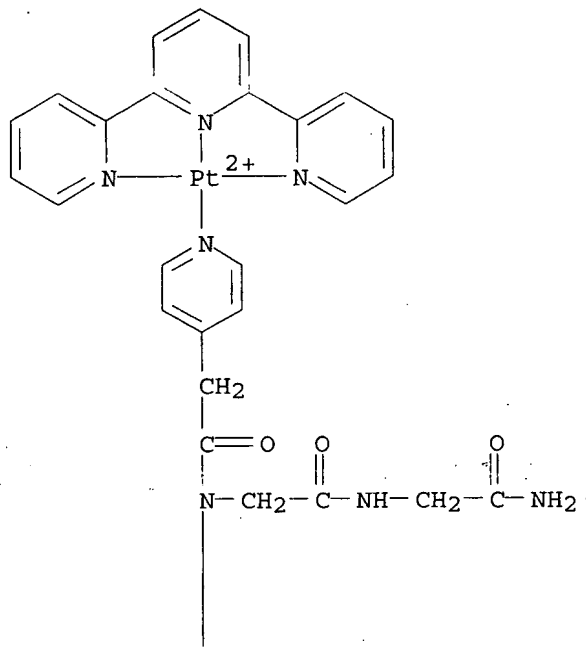


RN 869190-62-5 HCAPLUS
 CN Platinum(10+), [μ 5-[N-[4,10,16,22,28-pentaoxo-28-phenyl-6,12,18,24-tetrakis[(4-pyridinyl- κ N)acetyl]-3,6,9,12,15,18,21,24,27-nonaazaoctacos-1-yl]-N-[(4-pyridinyl- κ N)acetyl]glycylglycinamide]]pentakis(2,2':6',2''-terpyridine- κ N1, κ N1', κ N1'')penta-(9CI) (CA INDEX NAME)

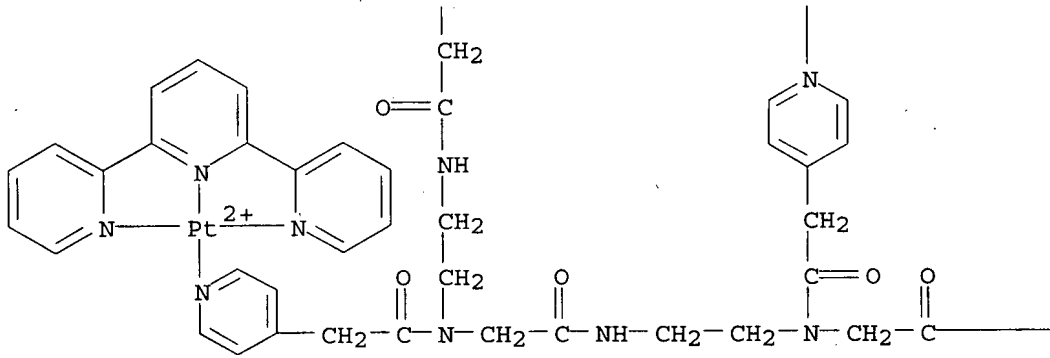
PAGE 1-A



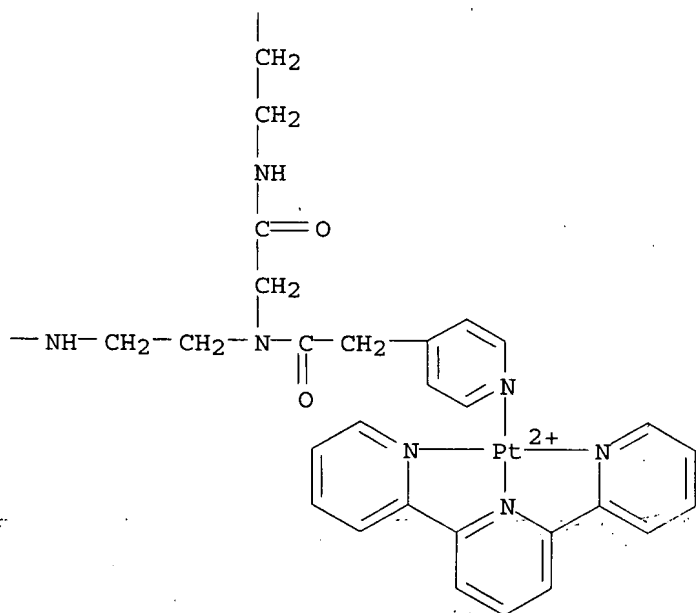
PAGE 1-B



PAGE 2-A

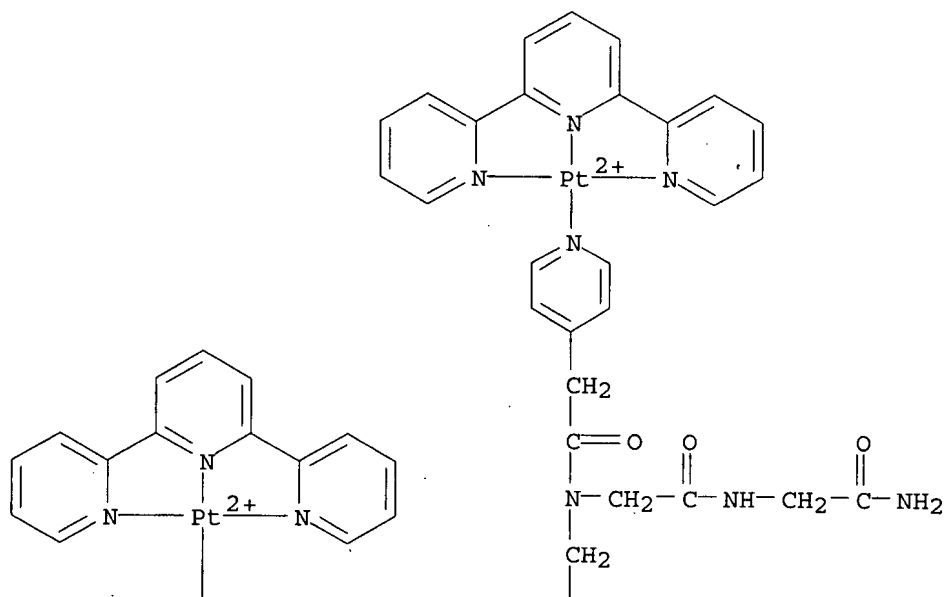


PAGE 2-B

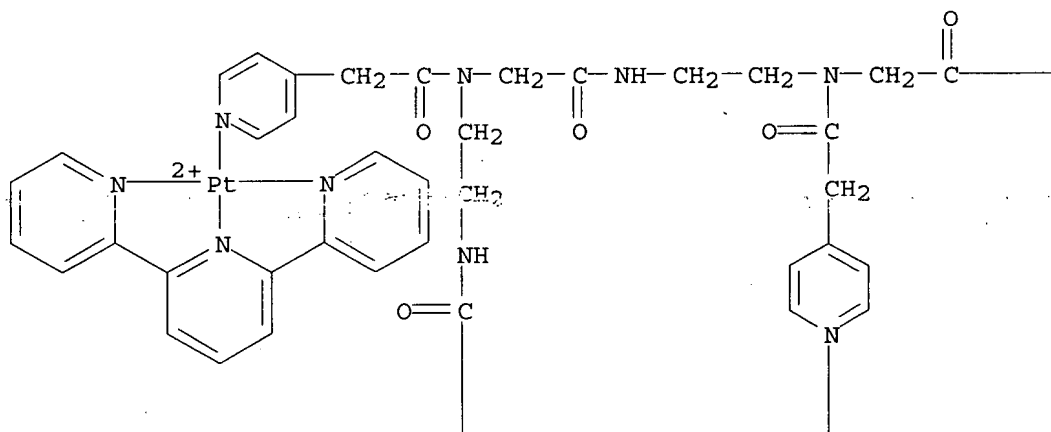


RN 869190-64-7 HCAPLUS
 CN Platinum(12+), [μ 6-[N-[4,10,16,22,28,34-hexaoxo-34-phenyl-6,12,18,24,30-pentakis[(4-pyridinyl- κ N)acetyl]-3,6,9,12,15,18,21,24,27,30,33-undecaazatetratriacont-1-yl]-N-[(4-pyridinyl- κ N)acetyl]glycylglycinamide]]hexakis(2,2':6',2''-terpyridine- κ N1, κ N1', κ N1'')hex
 a- (9CI) (CA INDEX NAME)

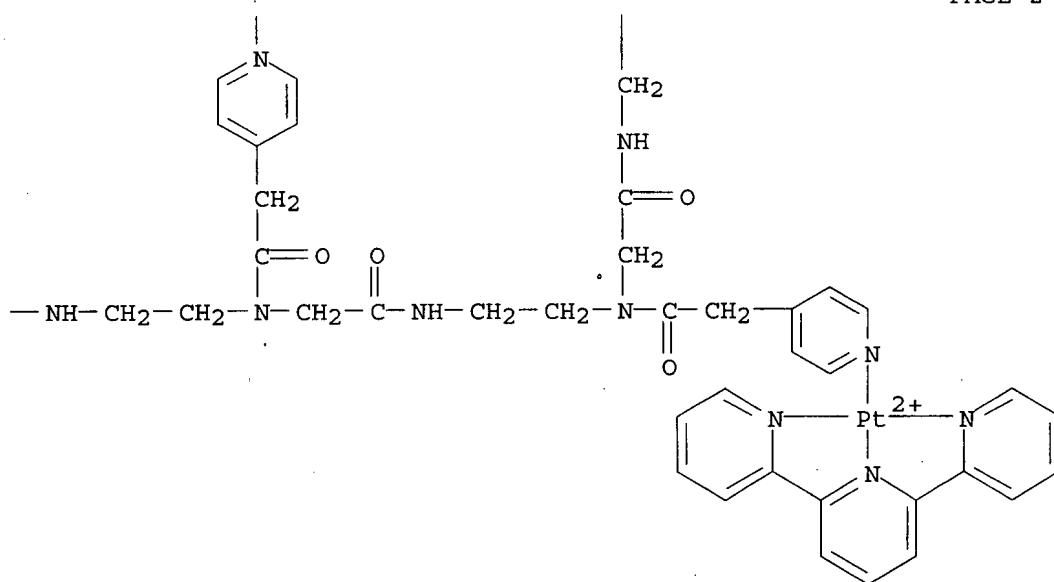
PAGE 1-B



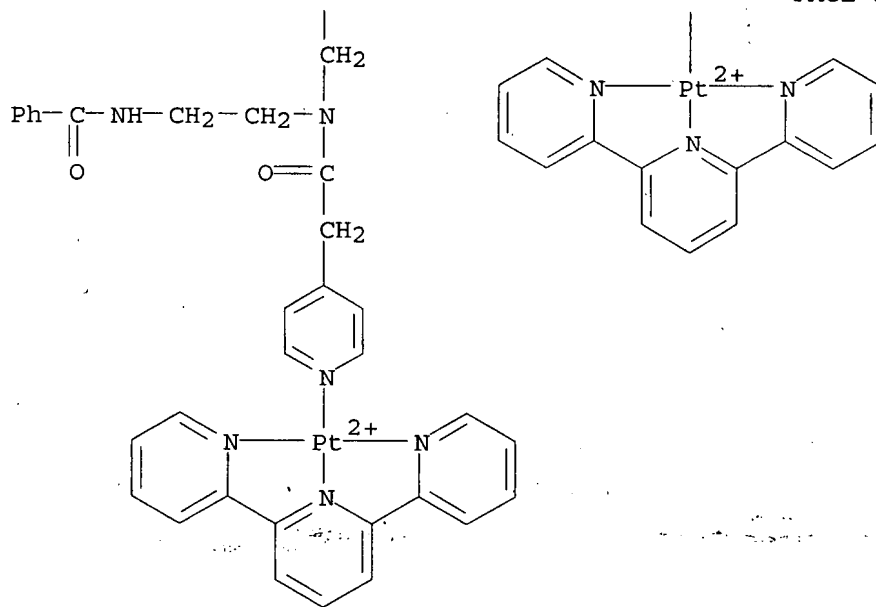
PAGE 2-A



PAGE 2-B



PAGE 3-A



IT 861886-02-4P 861886-04-6P 869190-49-8P

869190-50-1P 869190-51-2P 869190-53-4P

869190-55-6P 869190-57-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

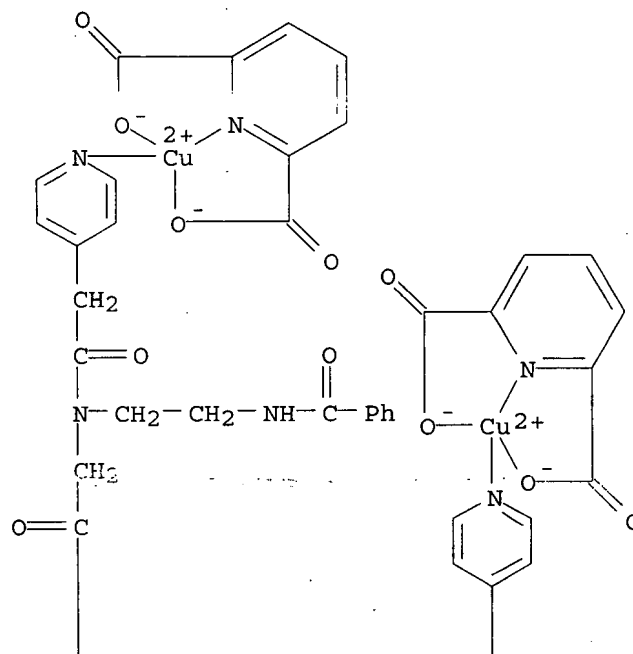
(preparation of pyridine-substituted oligopeptide scaffolds

coordinated with metal(II) chelates)

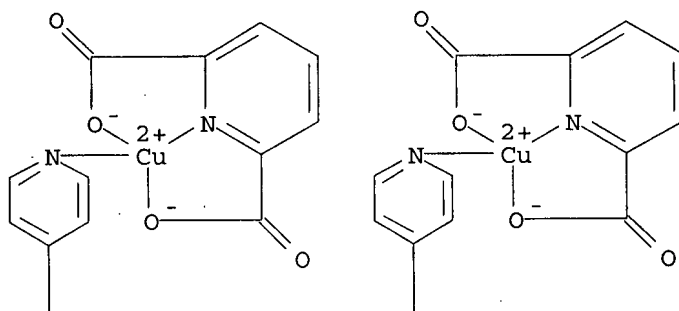
RN 861886-02-4 HCAPLUS

CN Copper, [μ_6 -[N-[4,10,16,22,28,34-hexaoxo-34-phenyl-6,12,18,24,30-pentakis[(4-pyridinyl- κ N)acetyl]-3,6,9,12,15,18,21,24,27,30,33-undecaazatetratriacont-1-yl]-N-[(4-pyridinyl- κ N)acetyl]glycylglycinamide]]hexakis[2,6-pyridinedicarboxylato(2-)- κ N1, κ O2, κ O6]hexa-, stereoisomer (9CI) (CA INDEX NAME)

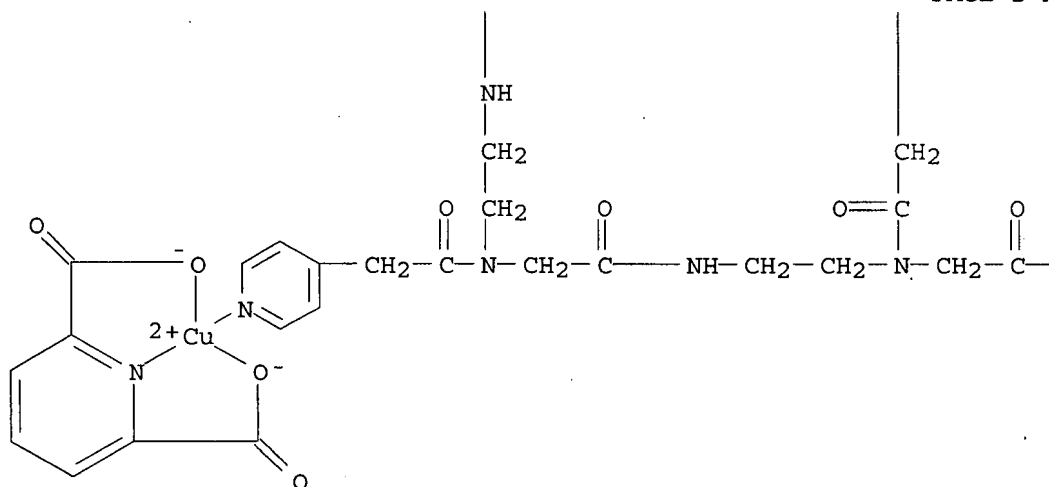
PAGE 1-A



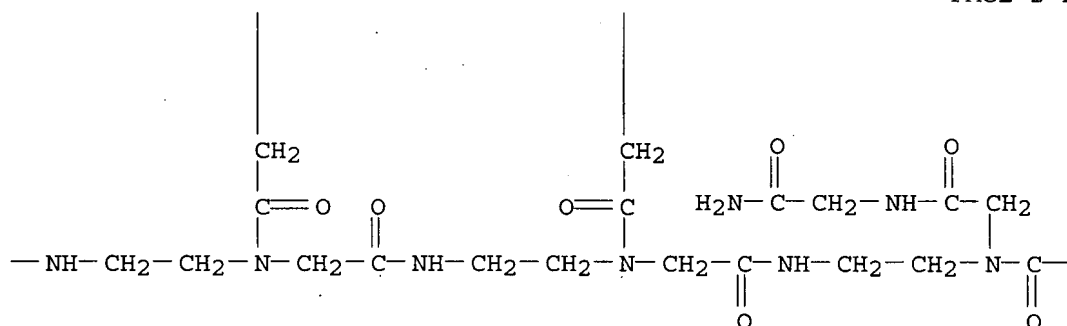
PAGE 1-B



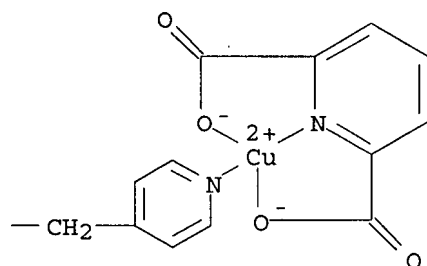
PAGE 2-A



PAGE 2-B



PAGE 2-C



RN 861886-04-6 HCAPLUS

CN Copper(12+), [μ_6 -[N-[4,10,16,22,28,34-hexaoxo-34-phenyl-6,12,18,24,30-pentakis[(4-pyridinyl- κ N)acetyl]-3,6,9,12,15,18,21,24,27,30,33-undecaazatetratriacont-1-yl]-N-[(4-pyridinyl- κ N)acetyl]glycylglycinamide]]hexakis(2,2':6',2''-terpyridine- κ N1, κ N1', κ N1'')hexa-, stereoisomer, dodecaperchlorate (9CI) (CA INDEX NAME)

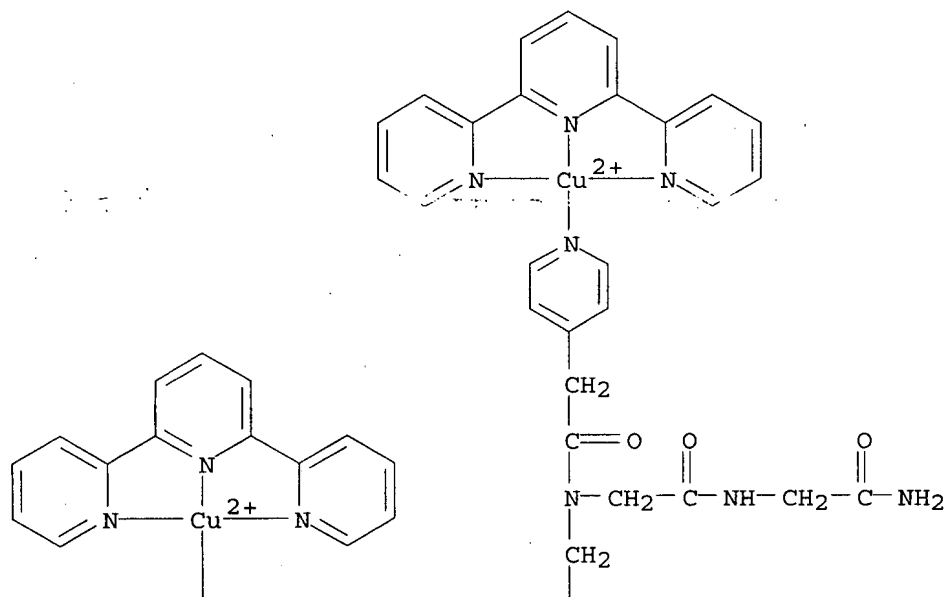
CM 1

CRN 861886-03-5

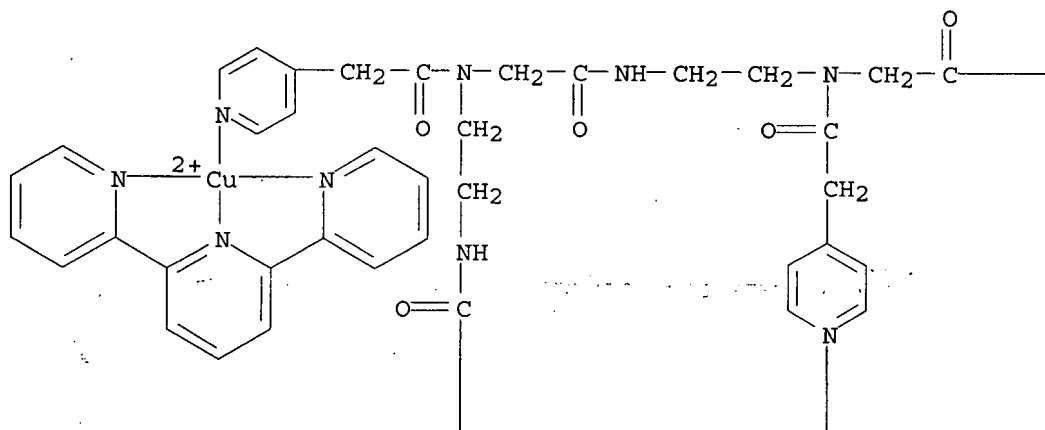
CMF C165 H154 Cu6 N38 O14

CCI CCS

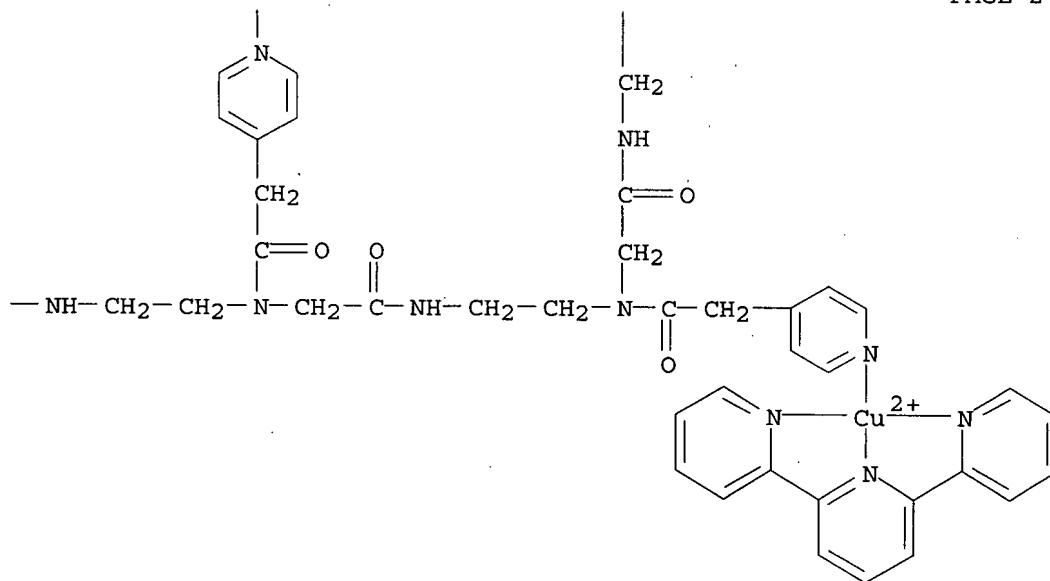
PAGE 1-B



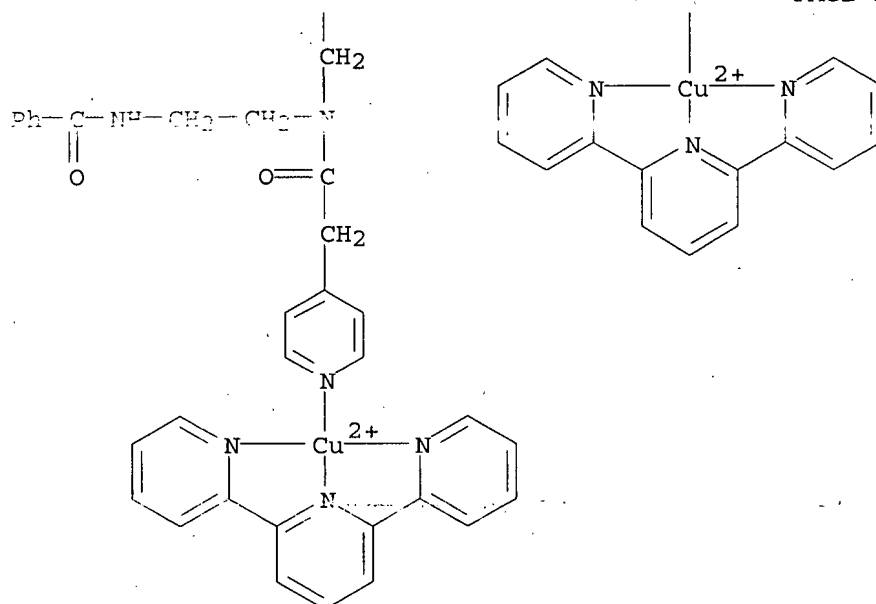
PAGE 2-A



PAGE 2-B



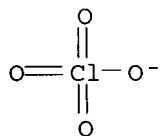
PAGE 3-A



CM 2

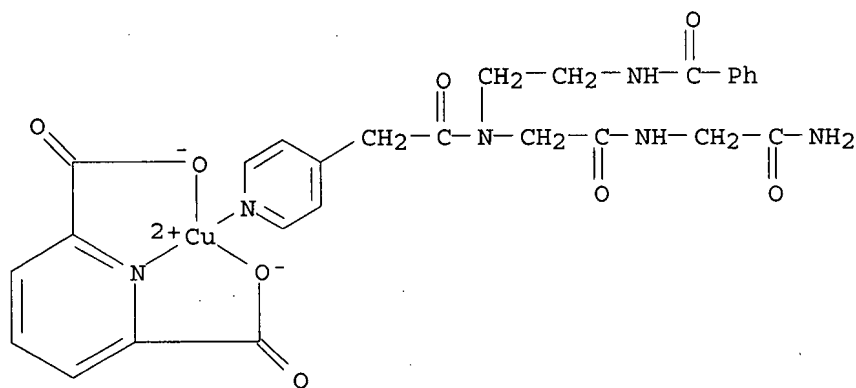
CRN 14797-73-0

CMF Cl O4



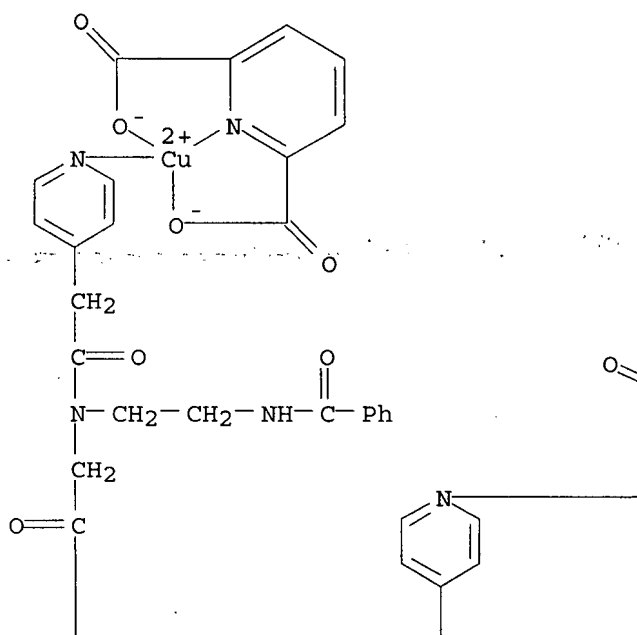
RN 869190-49-8 HCAPLUS

CN Copper, [N-[2-(benzoylamino)ethyl]-N-[(4-pyridinyl- κ N)acetyl]glycylglycinamide] [2,6-pyridinedicarboxylato(2-)- κ N1, κ O2, κ O6]-, (SP-4-1)- (9CI) (CA INDEX NAME)

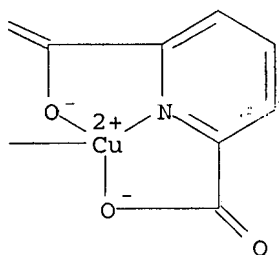


RN 869190-50-1 HCAPLUS
 CN Copper, tetrakis [2,6-pyridinedicarboxylato(2-)-
 $\kappa N1, \kappa O2, \kappa O6$] [$\mu 4$ - [N- [(4-pyridinyl- κN) acetyl] -N-
 [4,10,16,22-tetraoxo-22-phenyl-6,12,18-tris [(4-pyridinyl- κN) acetyl] -
 3,6,9,12,15,18,21-heptaazadocos-1-yl]glycylglycinamide]]tetra-,
 stereoisomer (9CI) (CA INDEX NAME)

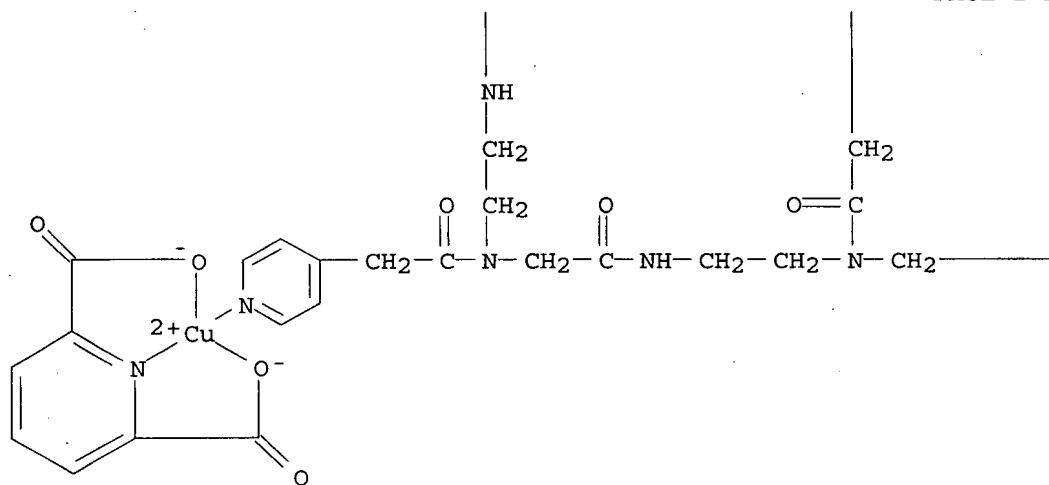
PAGE 1-A



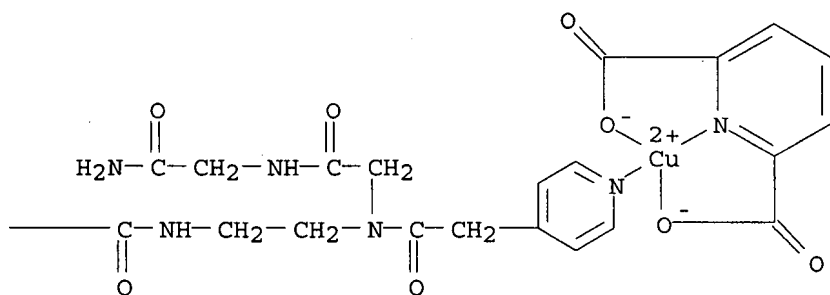
PAGE 1-B



PAGE 2-A



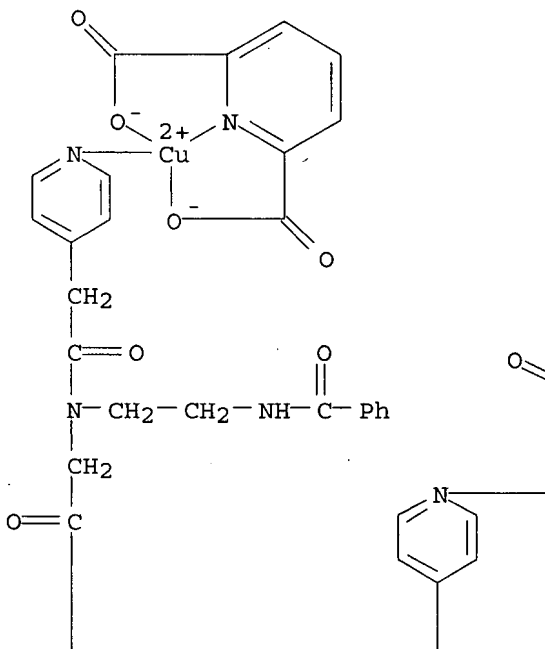
PAGE 2-B



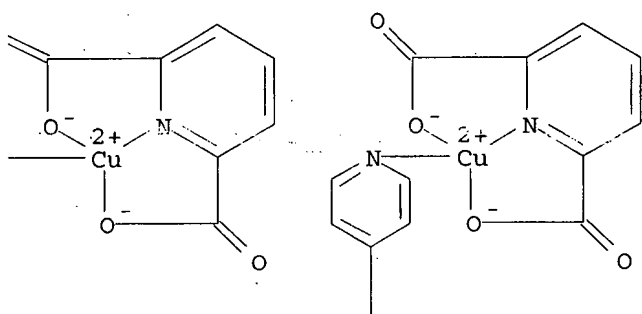
RN 869190-51-2 HCAPLUS

CN Copper, [μ 5-[N-[4,10,16,22,28-pentaoxo-28-phenyl-6,12,18,24-tetrakis[(4-pyridinyl- κ N)acetyl]-3,6,9,12,15,18,21,24,27-nonaazaoctacos-1-yl]-N-[(4-pyridinyl- κ N)acetyl]glycylglycinamide]]pentakis[2,6-pyridinedicarboxylato(2-)- κ N1, κ O2, κ O6]]penta-, stereoisomer (9CI) (CA INDEX NAME)

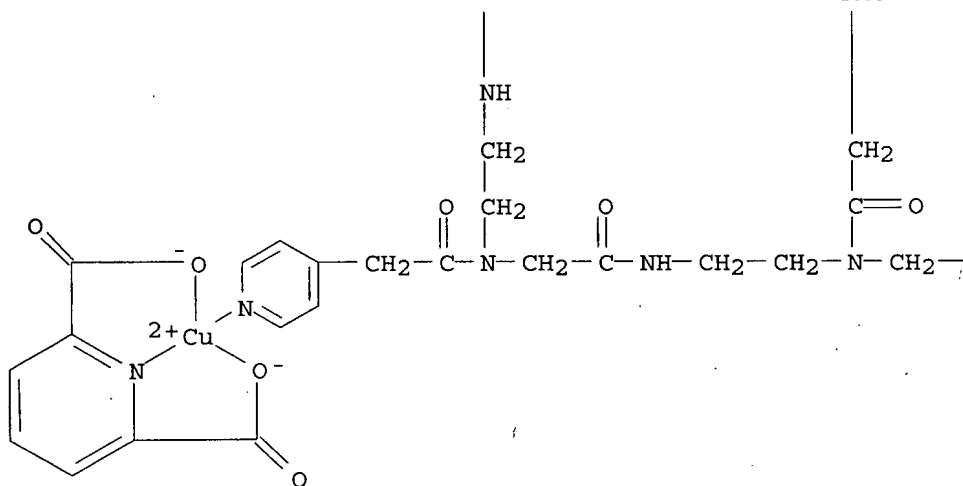
PAGE 1-A



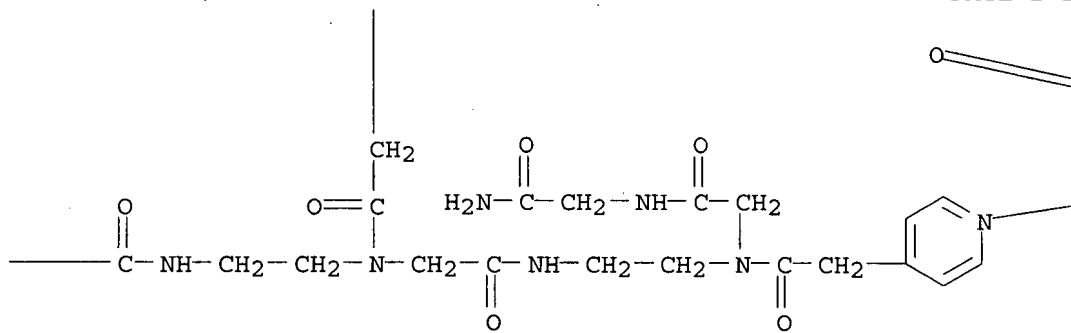
PAGE 1-B



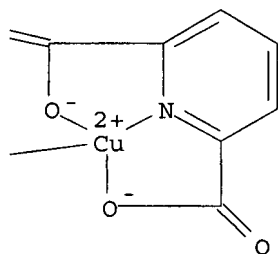
PAGE 2-A



PAGE 2-B



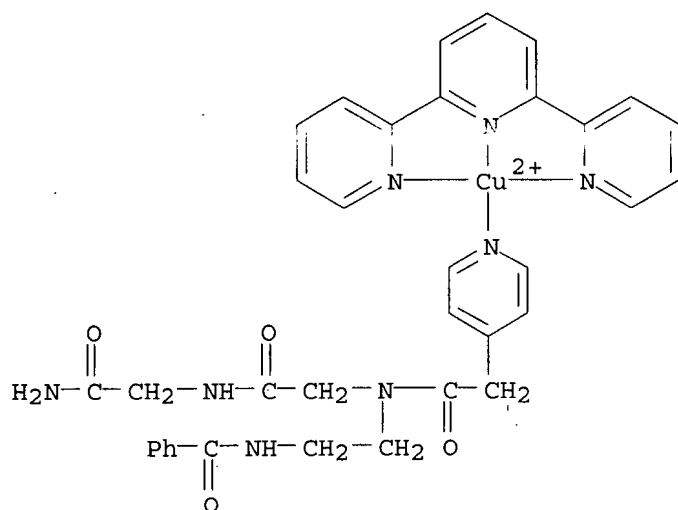
PAGE 2-C



RN	869190-53-4	HCAPLUS
CN	Copper(2+), [N-[2-(benzoylamino)ethyl]-N-[(4-pyridinyl-κN)acetyl]glycylglycinamide](2,2':6',2''-terpyridine-κN1,κN1',κN1'')-, (SP-4-3)-, diperchlorate (9CI) (CA INDEX NAME)	

CM 1

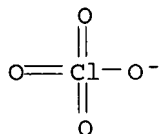
CRN 869190-52-3
CMF C35 H34 Cu N8 O4
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



RN 869190-55-6 HCAPLUS

CN Copper(8+), [μ₄-[N-[(4-pyridinyl-κN)acetyl]-N-[4,10,16,22-tetraoxo-22-phenyl-6,12,18-tris[(4-pyridinyl-κN)acetyl]-3,6,9,12,15,18,21-heptaazadocos-1-yl]glycylglycinamide]]tetrakis(2,2':6',2''-terpyridine-κN1,κN1',κN1'')tetra-, stereoisomer, octaperchlorate (9CI) (CA INDEX NAME)

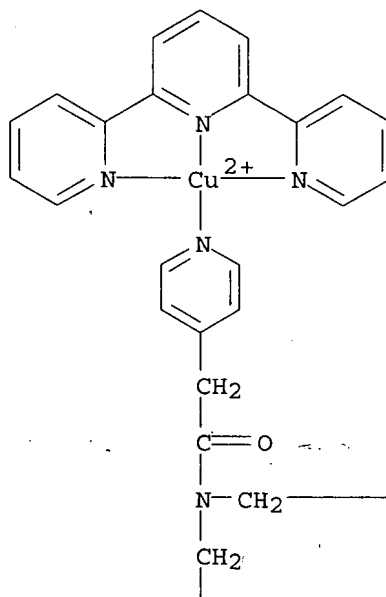
CM 1

CRN 869190-54-5

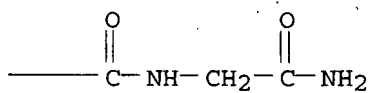
CMF C113 H106 Cu4 N26 O10

CCI CCS

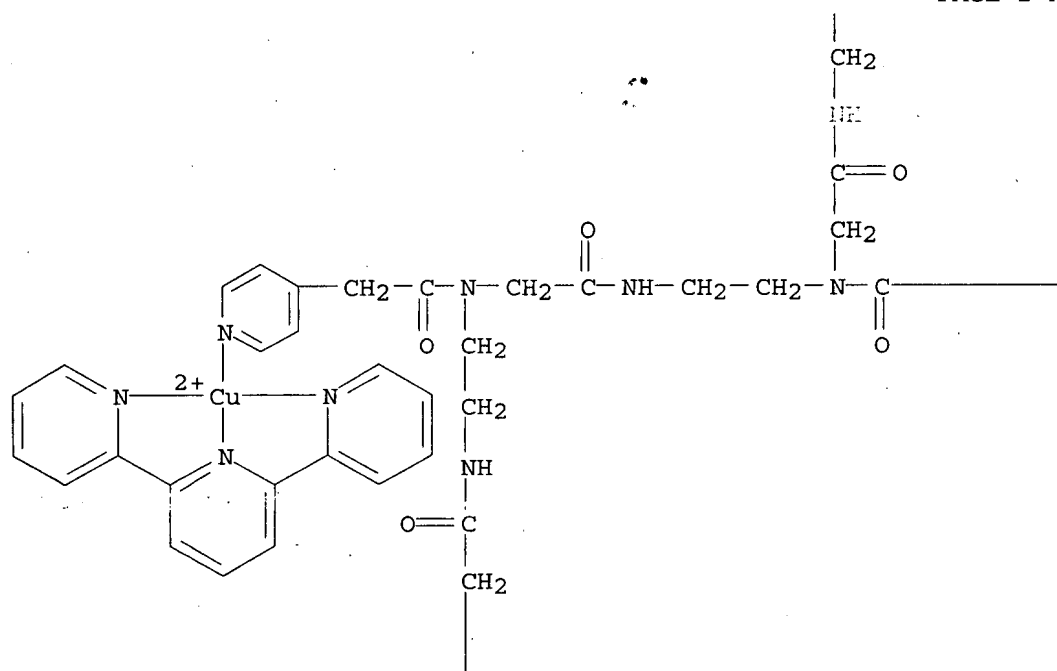
PAGE 1-A



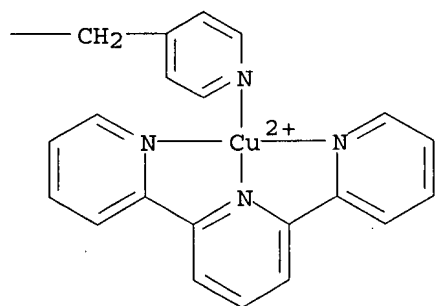
PAGE 1-B



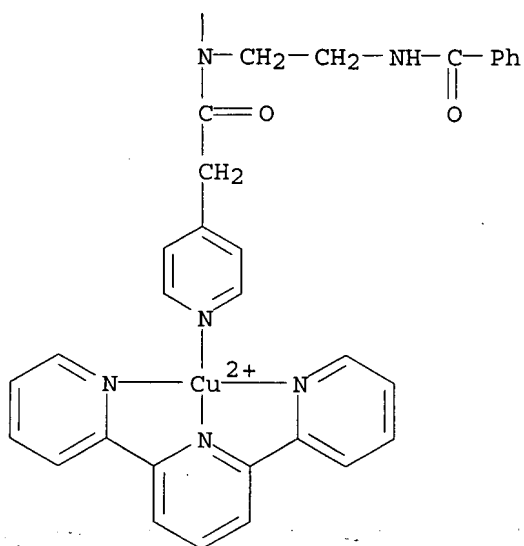
PAGE 2-A



PAGE 2-B



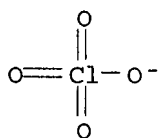
PAGE 3-A



CM 2

CRN 14797-73-0

CMF Cl O4



RN 869190-57-8 HCAPLUS

CN Copper(10+), [μ 5-[N-[4,10,16,22,28-pentaoxo-28-phenyl-6,12,18,24-tetrakis[(4-pyridinyl- κ N)acetyl]-3,6,9,12,15,18,21,24,27-nonaazaocacos-1-yl]-N-[(4-pyridinyl- κ N)acetyl]glycylglycinamide]]pentakis(2,2':6',2''-terpyridine- κ N1, κ N1', κ N1'')penta-, stereoisomer, decaperchlorate (9CI) (CA INDEX NAME)

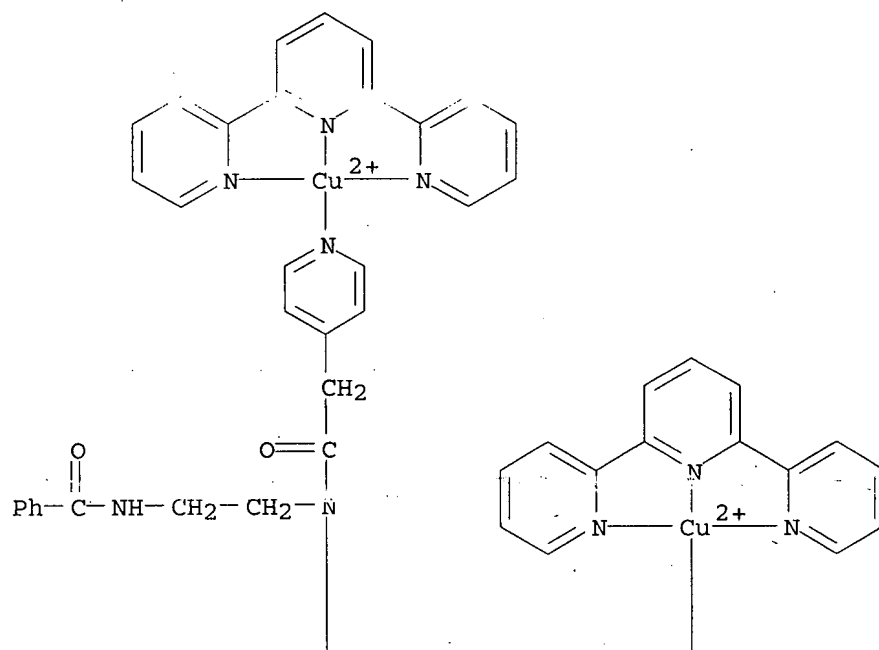
CM 1

CRN 869190-56-7

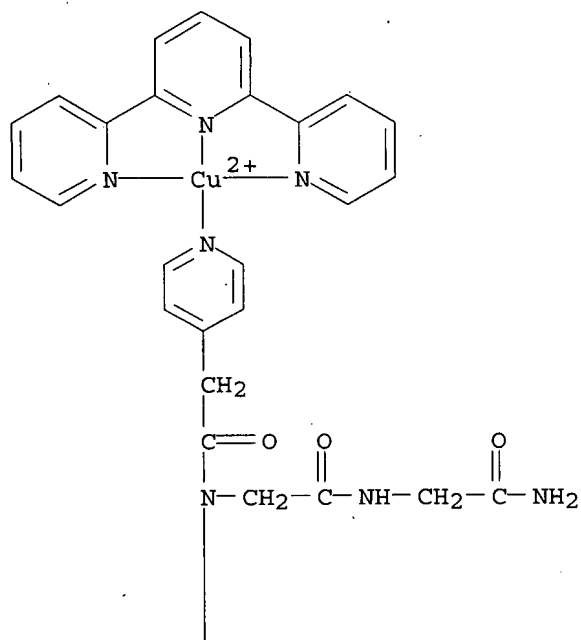
CMF C139 H130 Cu5 N32 O12

CCI CCS

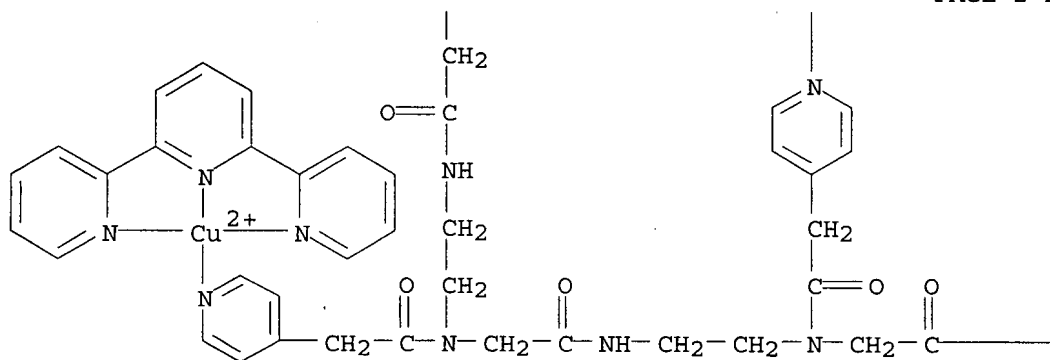
PAGE 1-A



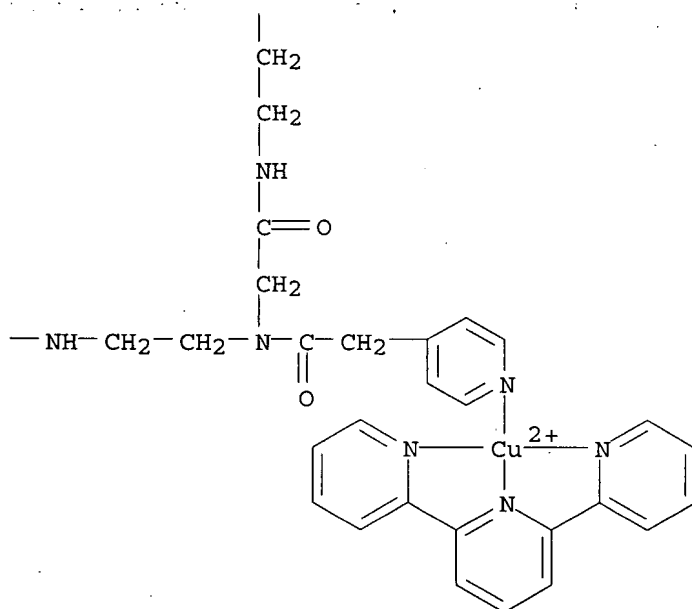
PAGE 1-B



PAGE 2-A

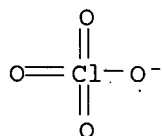


PAGE 2-B



CM 2

CRN 14797-73-0
CMF C1 O4



IT 869190-59-0P 869190-61-4P 869190-63-6P
869190-65-8P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(preparation, cyclic voltammetry, and diffusion coefficient measured with chronoamperometry)

869190-58-9 HCAPLUS

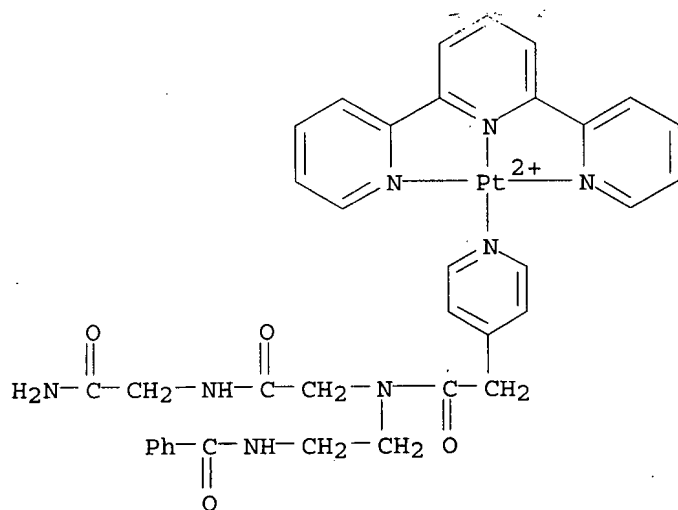
CN Platinum(2+), [N-[2-(benzoylamino)ethyl]-N-[(4-pyridinyl- κ N)acetyl]glycylglycinamide] (2,2':6',2''-terpyridine- κ N1, κ N1', κ N1'')-, (SP-4-3)-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 869190-58-9

CMF C35 H34 N8 O4 Pt

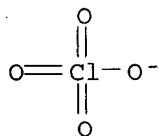
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



RN 869190-61-4 HCAPLUS

CN Platinum(8+), [μ 4-[N-[(4-pyridinyl- κ N)acetyl]-N-[4,10,16,22-tetraoxo-22-phenyl-6,12,18-tris[(4-pyridinyl- κ N)acetyl]-3,6,9,12,15,18,21-heptaazadocos-1-yl]glycylglycinamide]]tetrakis(2,2':6',2''-terpyridine- κ N1, κ N1', κ N1'')tetra-, octaperchlorate (9CI) (CA INDEX NAME)

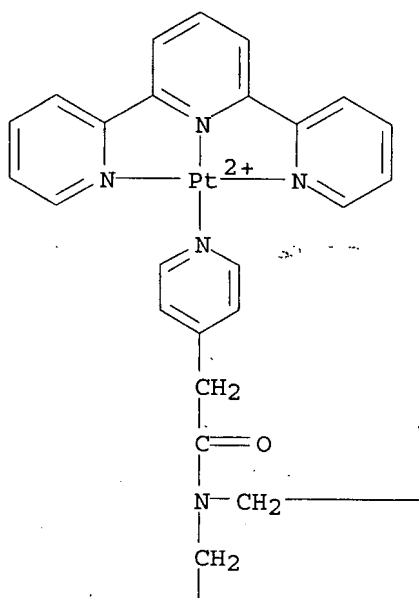
CM 1

CRN 869190-60-3

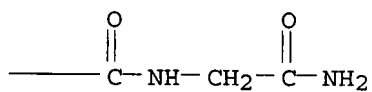
CMF C113 H106 N26 O10 Pt4

CCI CCS

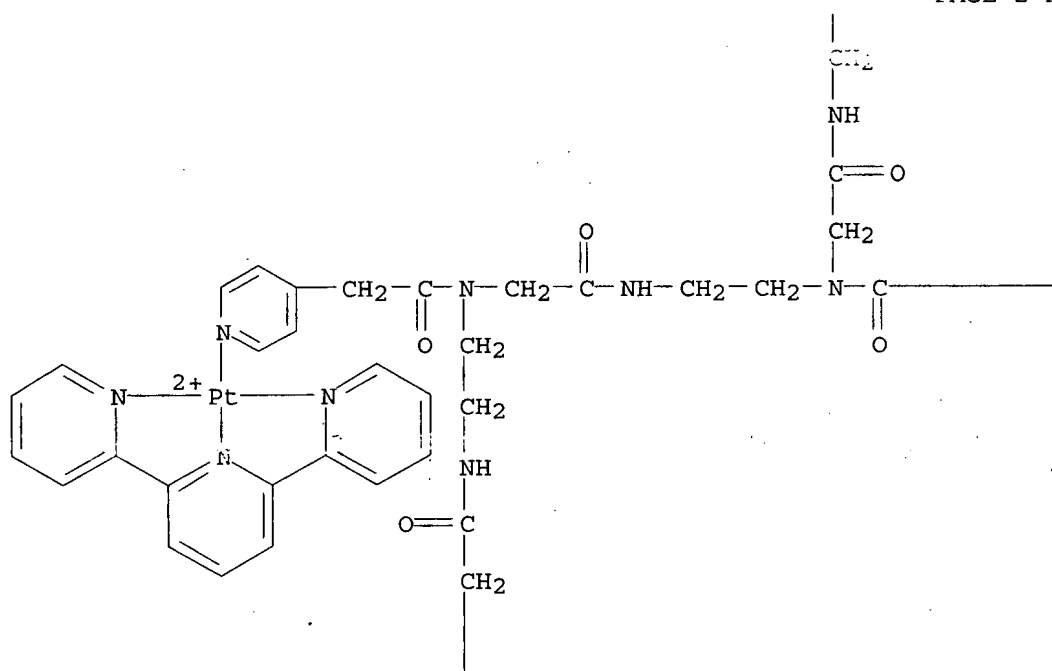
PAGE 1-A



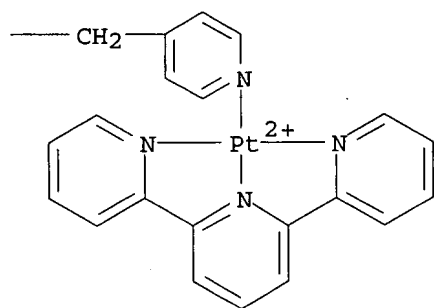
PAGE 1-B



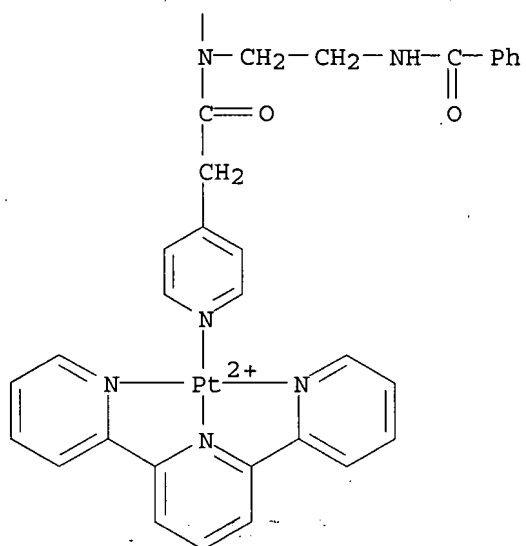
PAGE 2-A



PAGE 2-B



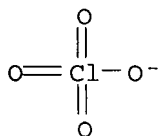
PAGE 3-A



CM 2

CRN 14797-73-0

CMF Cl O4



RN 869190-63-6 HCAPLUS

CN Platinum(10+), [μ5-[N-[4,10,16,22,28-pentaoxo-28-phenyl-6,12,18,24-tetrakis[(4-pyridinyl-κN)acetyl]-3,6,9,12,15,18,21,24,27-nonaazaoctacos-1-yl]-N-[(4-pyridinyl-κN)acetyl]glycylglycinamide]]pentakis(2,2':6',2''-terpyridine-κN1,κN1',κN1'')penta-, decaperchlorate (9CI) (CA INDEX NAME)

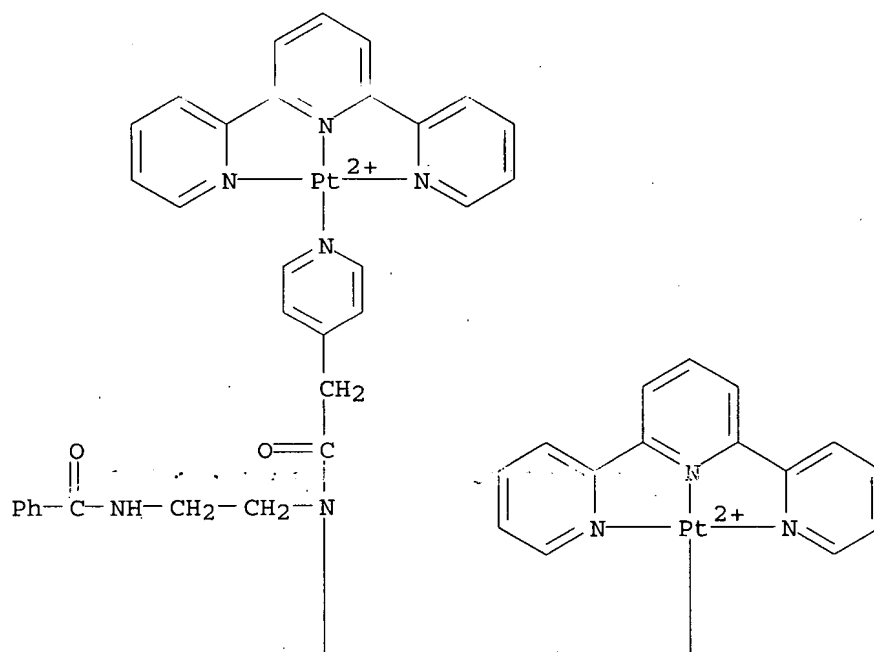
CM 1

CRN 869190-62-5

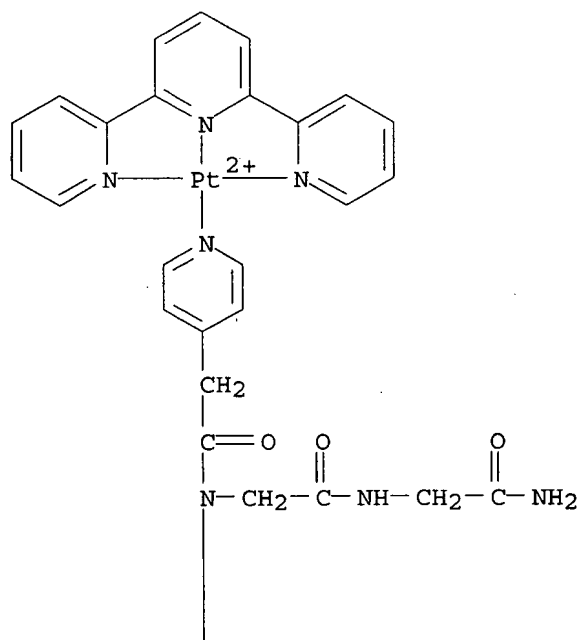
CMF C139 H130 N32 O12 Pt5

CCI CCS

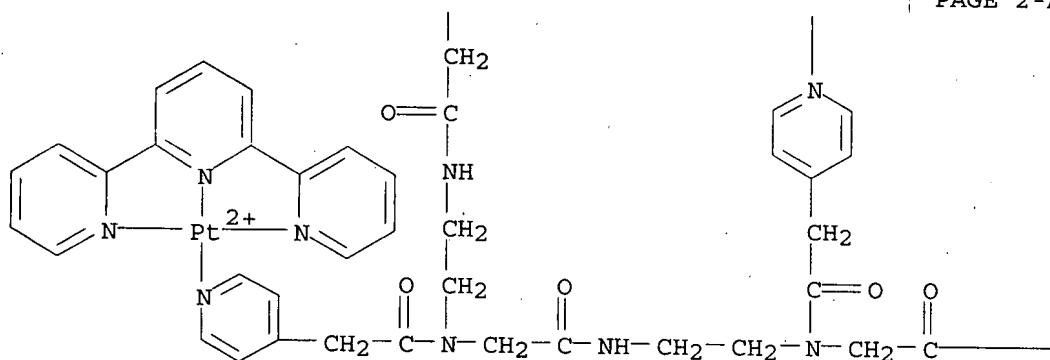
PAGE 1-A



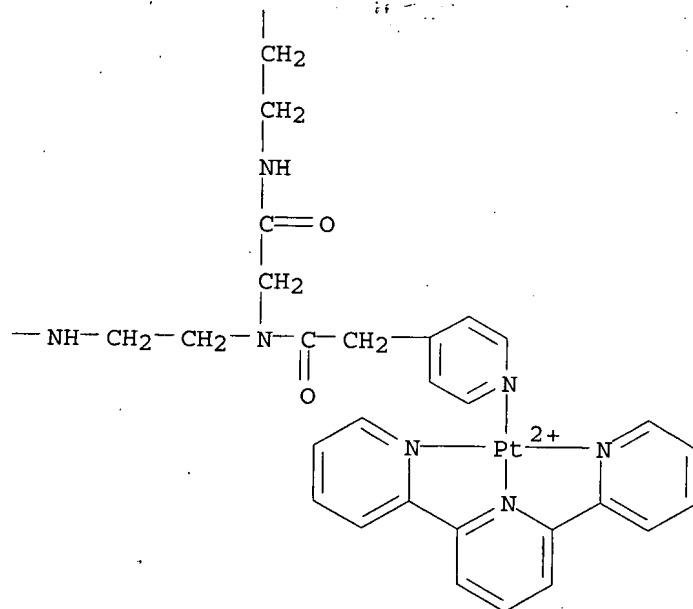
PAGE 1-B



PAGE 2-A



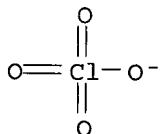
PAGE 2-B



CM 2

CRN 14797-73-0
CMF C1 O4

CMF C1 O4



RN 869190-65-8 HCAPLUS

CN Platinum(12+), [μ6-[N-[4,10,16,22,28,34-hexaoxo-34-phenyl-6,12,18,24,30-

pentakis[(4-pyridinyl- κ N)acetyl]-3,6,9,12,15,18,21,24,27,30,33-undecaazatetratriacont-1-yl]-N-[(4-pyridinyl- κ N)acetyl]glycylglycinamide]]hexakis(2,2':6',2''-terpyridine- κ N1, κ N1', κ N1'')hexa-, dodecaperchlorate (9CI) (CA INDEX NAME)

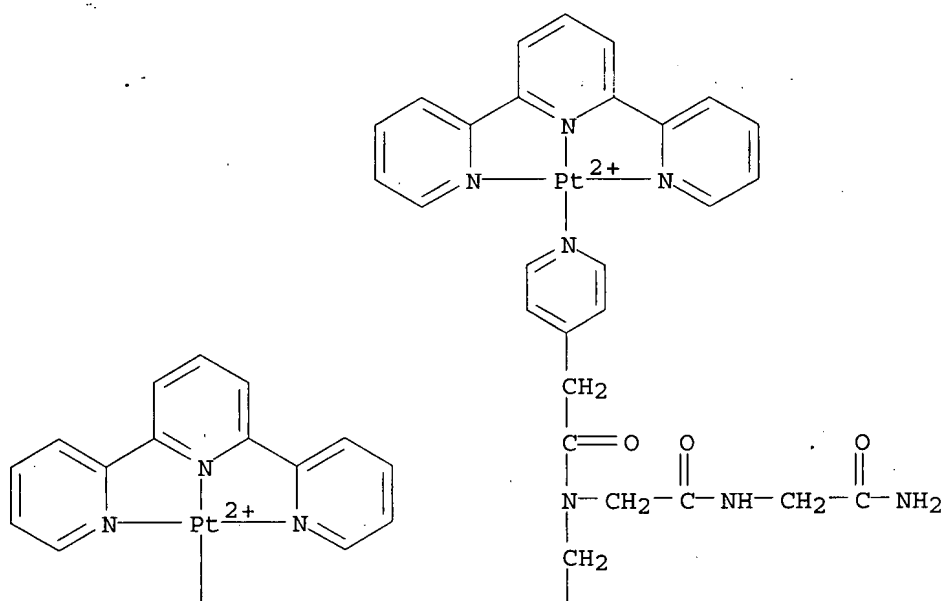
CM 1

CRN 869190-64-7

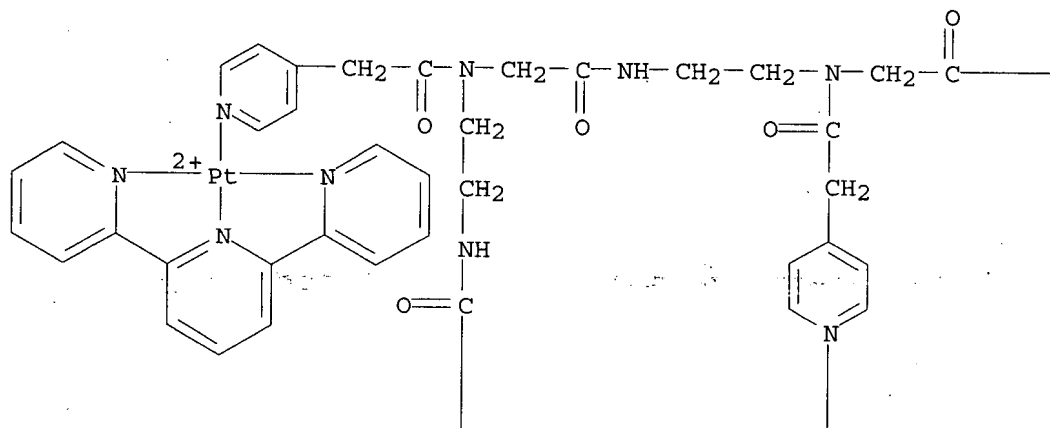
CMF C165 H154 N38 O14 Pt6

CCI CCS

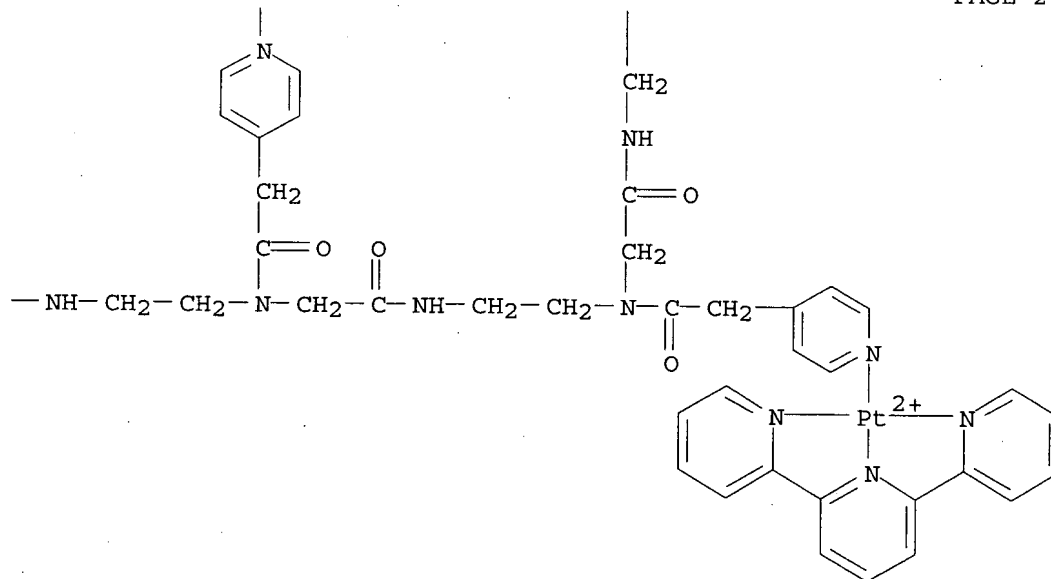
PAGE 1-B



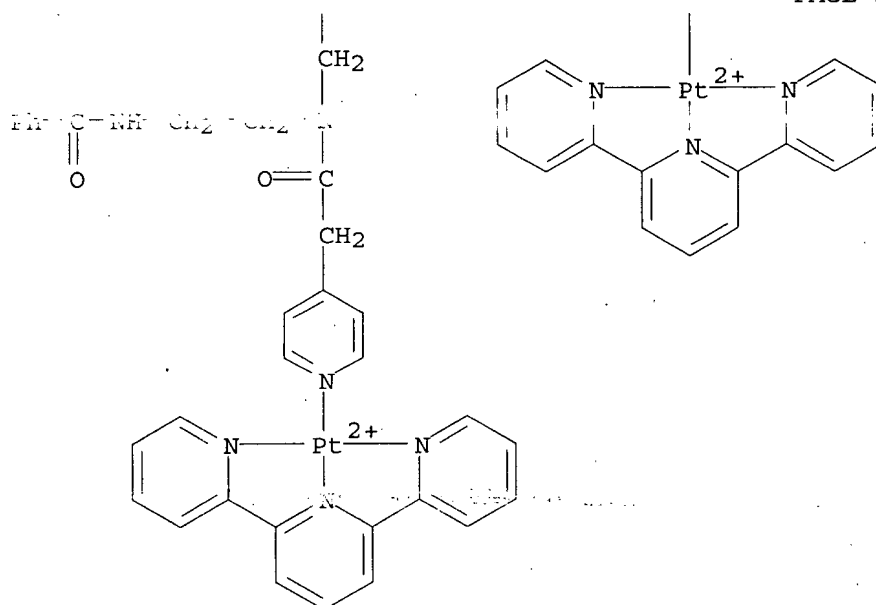
PAGE 2-A



PAGE 2-B



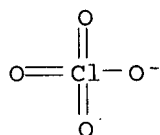
PAGE 3-A



CM 2

CRN 14797-73-0

CMF C1 04



L74 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:508556 HCAPLUS

DOCUMENT NUMBER: 143:205125

TITLE: Artificial **Oligopeptide** Scaffolds for
Stoichiometric Metal Binding

AUTHOR(S) : Gilmartin, Brian P.; Ohr, Kristi; McLaughlin, Rebekah L.; Koerner, Richard; Williams, Mary Elizabeth

CORPORATE SOURCE: Department of Chemistry, Pennsylvania State University, University Park, PA, 16802, USA

SOURCE: Journal of the American Chemical Society (2005),
127(26), 9546-9555
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S) : CASREACT 143:205125

AB Two artificial **peptides** with pendant pyridine or bipyridine ligands were synthesized and incorporated into oligomeric strands that are

analogous to **peptide** nucleic acid. Spectrophotometric titrns. with Cu^{2+} and Fe^{2+} show that the oligomers bind stoichiometric quantities of **transition metals** based on the number of pendant ligands. The identities of the titration products are confirmed by high resolution **mass spectrometry**. In the case of the bipyridine **tripeptides**, the titration stoichiometry and mass spectra indicate that the metal ions form interstrand cross-links between two **oligopeptides**, creating duplex structures linked exclusively by metal ions. Calculated mol. structures of the metalated **oligopeptides** and duplexes indicate that the **peptide** backbone acts as a scaffold for the directed assembly of metal ions. ESR spectroscopy of the Cu-containing mols. have varying degrees of electronic interaction based on their charge and supramol. structure. Cyclic voltammetry of the Fe^{2+} - and Cu^{2+} -linked bipy **oligopeptide** duplexes shows that they possess unique electrochem. signatures based on the redox reactivity of the metal complex.

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 34, 72, 77

ST **oligopeptide** scaffold prepn stoichiometric complexation **transition metal**; copper artificial **oligopeptide** scaffold prepn EPR cyclic voltammetry; iron artificial **oligopeptide** scaffold prepn cyclic voltammetry; mol structure calcn copper **oligopeptide** scaffold complex

IT Redox reaction

(electrochem.; of copper(II) and iron(II) complexes of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands)

IT Molecular structure

(energy-minimized; of hexanuclear copper(II) pyridinedicarboxylate **hexapeptide** complex and bipyridine **tripeptide** duplex from mol. modeling)

IT ESR (electron spin resonance)

(of copper(II) complexes of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands)

IT Molecular modeling

(of hexanuclear copper(II) pyridinedicarboxylate **hexapeptide** complex and bipyridine **tripeptide** duplex)

IT **Transition metal** complexes

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (**peptide**; preparation of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))

IT **Oligopeptides**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))

IT **Oligopeptides**

Peptides, preparation

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (**transition metal** complexes; preparation of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))

IT 6622-91-9, 4-Pyridylacetic acid hydrochloride

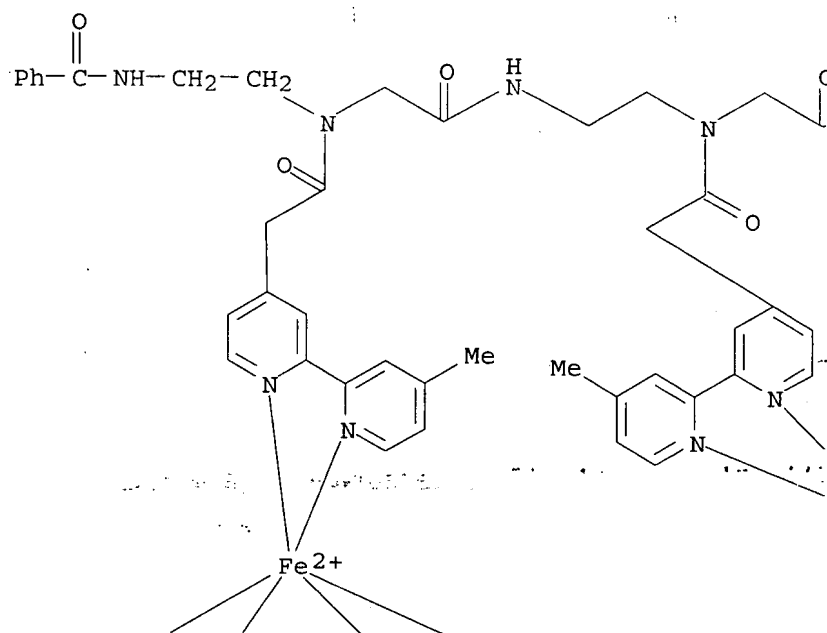
RL: RCT (Reactant); RACT (Reactant or reagent) (for preparation of **hexapeptide** bearing pyridines)

IT 861885-96-3P

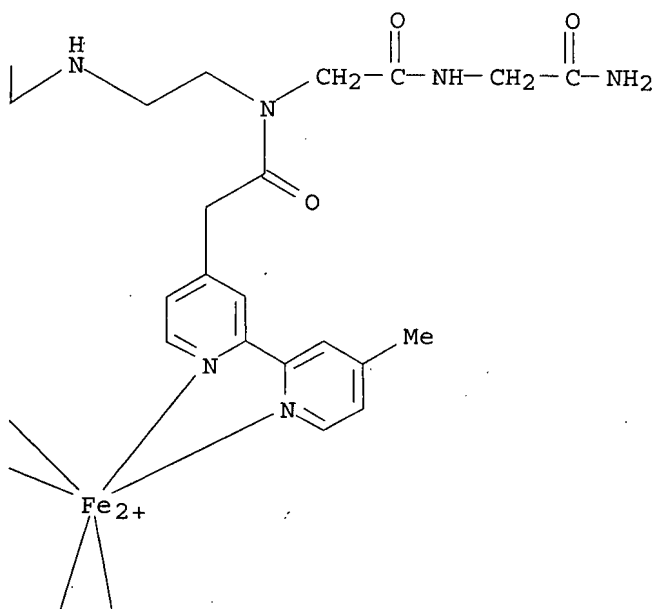
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

- (Reactant or reagent)
(for preparation of **hexapeptide** bearing pyridines and subsequent binding to **transition metal** ions)
- IT 169396-88-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of **oligopeptides** bearing pyridines or bipyridines and subsequent binding to **transition metal** ions)
- IT 118724-25-7, 4'-Methyl-2,2'-bipyridine-4-acetic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of **tripeptide** bearing bipyridines and subsequent binding to **transition metal** ions)
- IT 861885-97-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of **tripeptide** bearing bipyridines and subsequent binding to **transition metal** ions)
- IT 861886-05-7P 861886-06-8P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))
- IT 861886-02-4P 861886-04-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))
- IT 93-97-0, Benzoic anhydride 29022-11-5, Fmoc-Gly-OH 105047-45-8
160400-58-8 861886-00-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))
- IT 7439-89-6DP, Iron, dinuclear duplex complex of **tripeptide** with pendant bipyridines 7440-50-8DP, Copper, trinuclear duplex complex of **tripeptide** with pendant bipyridines 861885-98-5P
861885-99-6DP, copper(II) and iron(II) duplex complexes 861885-99-6P
861886-01-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))
- IT 861886-05-7P 861886-06-8P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))
- RN 861886-05-7 HCAPLUS
CN Iron(4+), bis[μ-[N-[6,12-bis[(4'-methyl[2,2'-bipyridin]-4-yl-κN1,κN1')acetyl]-4,10,16-trioxo-16-phenyl-3,6,9,12,15-pentaazahexadec-1-yl]-N-[(4'-methyl[2,2'-bipyridin]-4-yl-κN1,κN1')acetyl]glycylglycinamide]di- (9CI) (CA INDEX NAME)

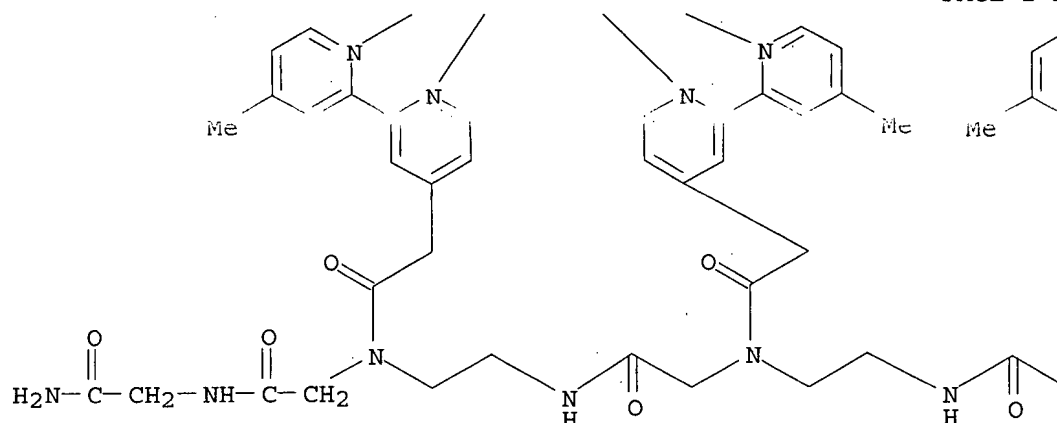
PAGE 1-A



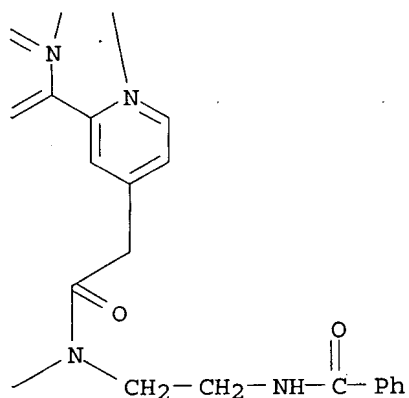
PAGE 1-B



PAGE 2-A

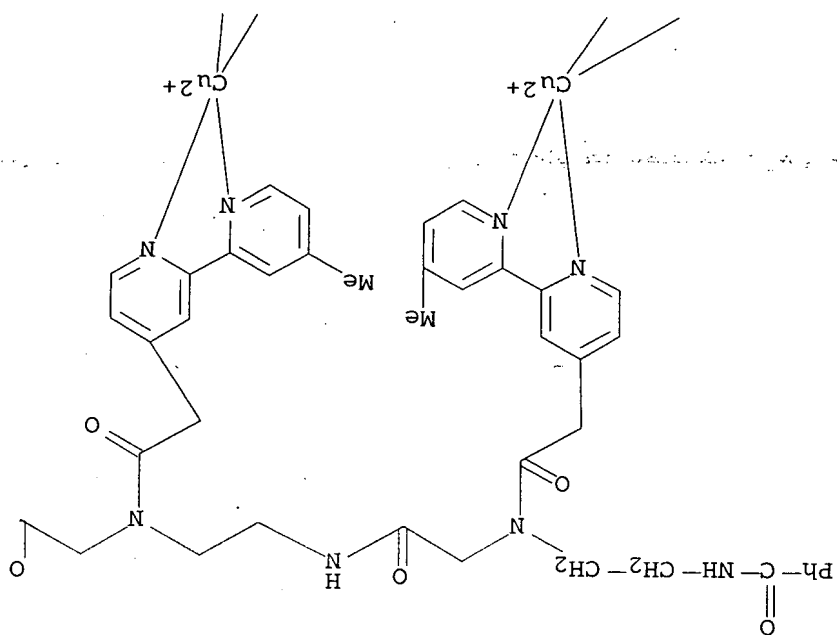


PAGE 2-B

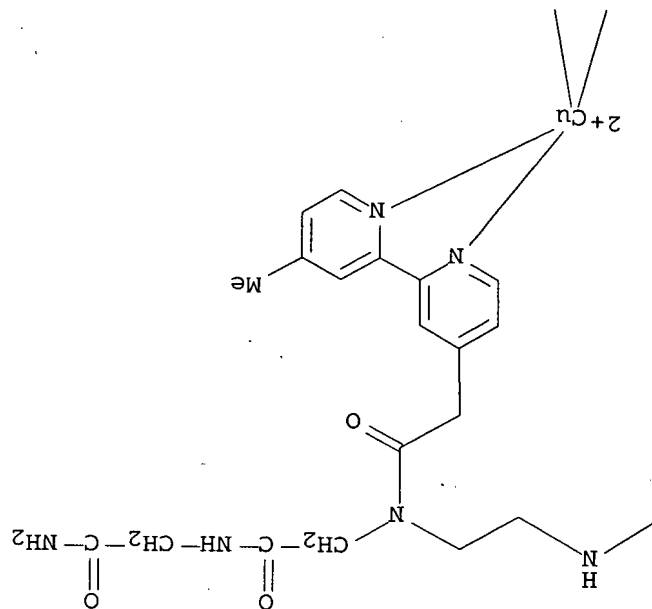


RN 861886-06-8 HCAPLUS
 CN Copper(6+), bis[μ3-[N-[6,12-bis[(4'-methyl[2,2'-bipyridin]-4-yl-κN1,κN1')acetyl]-4,10,16-trioxo-16-phenyl-3,6,9,12,15-pentaazahexadec-1-yl]-N-[(4'-methyl[2,2'-bipyridin]-4-yl-κN1,κN1')acetyl]glycylglycinamide]tri-, stereoisomer (9CI)
 (CA INDEX NAME)

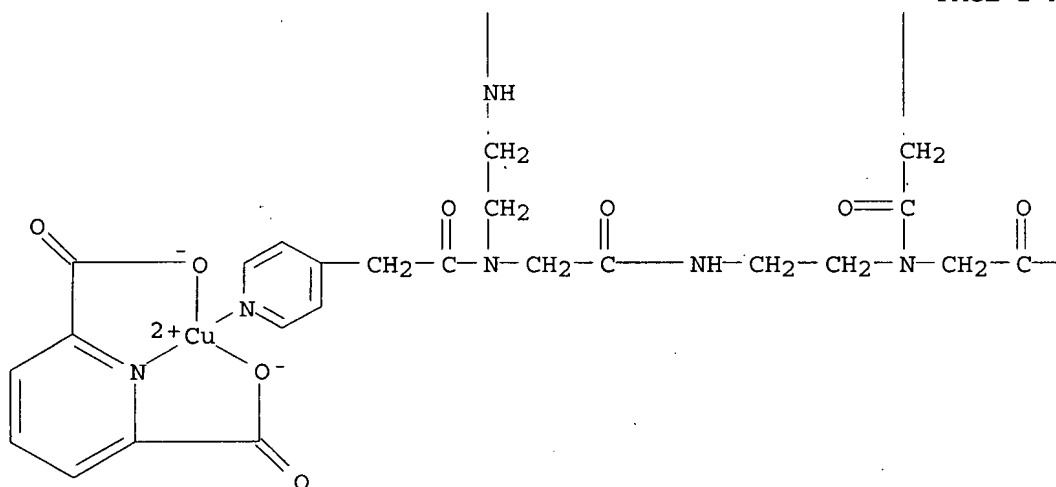
PAGE 1-A



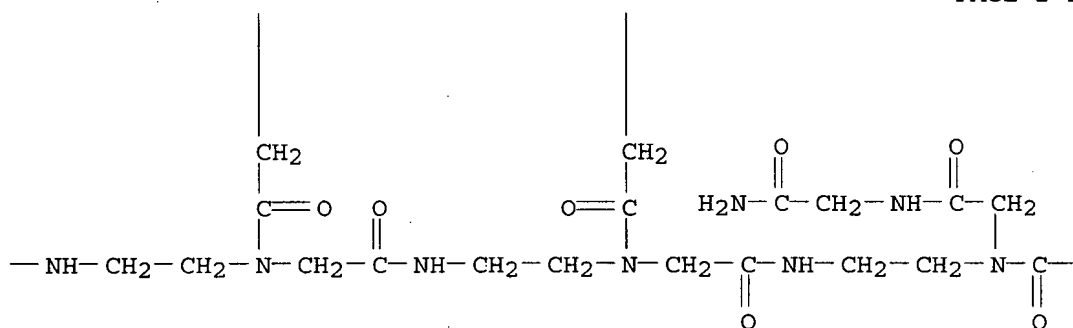
PAGE 1-B



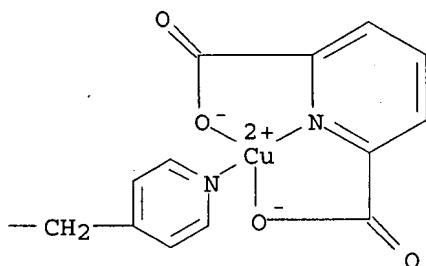
PAGE 2-A



PAGE 2-B



PAGE 2-C

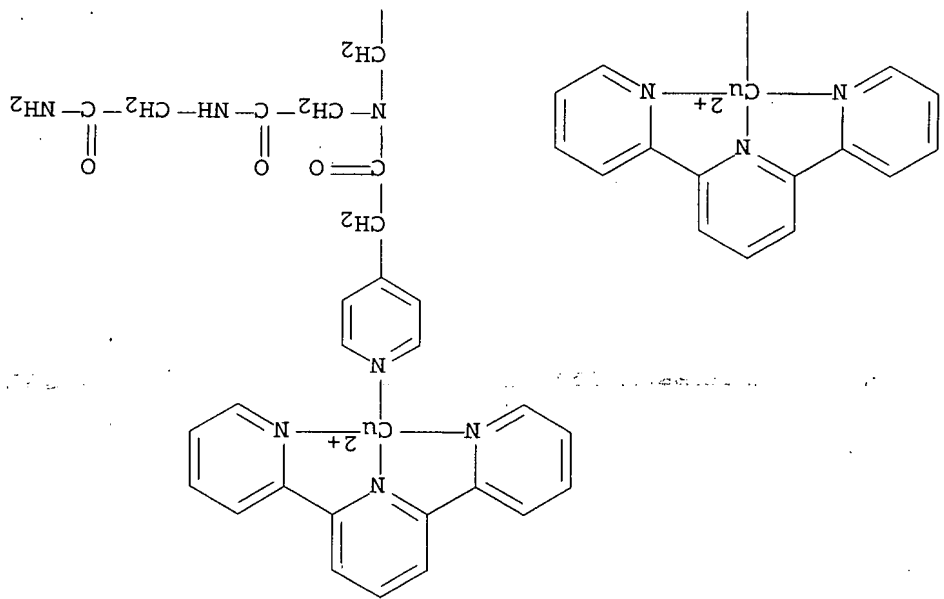


RN 861886-04-6 HCAPLUS

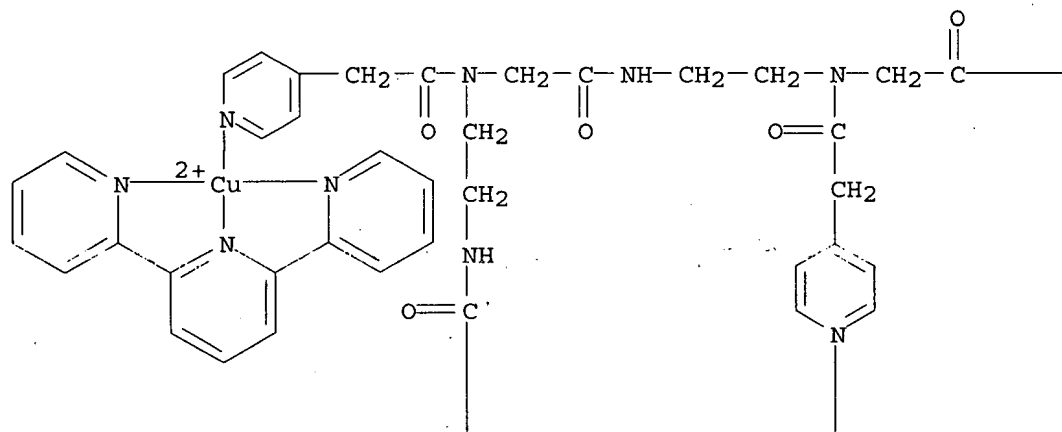
CN Copper(12+), [μ_6 -[N-[4,10,16,22,28,34-hexaoxo-34-phenyl-6,12,18,24,30-pentakis[(4-pyridinyl- κ N)acetyl]-3,6,9,12,15,18,21,24,27,30,33-undecaazatetratriacont-1-yl]-N-[(4-pyridinyl- κ N)acetyl]glycylglycinamide]]hexakis(2,2':6',2''-terpyridine- κ N1, κ N1', κ N1'')hexa-, stereoisomer, dodecaperchlorate (9CI) (CA INDEX NAME)

CM 1
 CRN 861886-03-5
 CMF C165 H154 Cu6 N38 O14
 CCI CCS

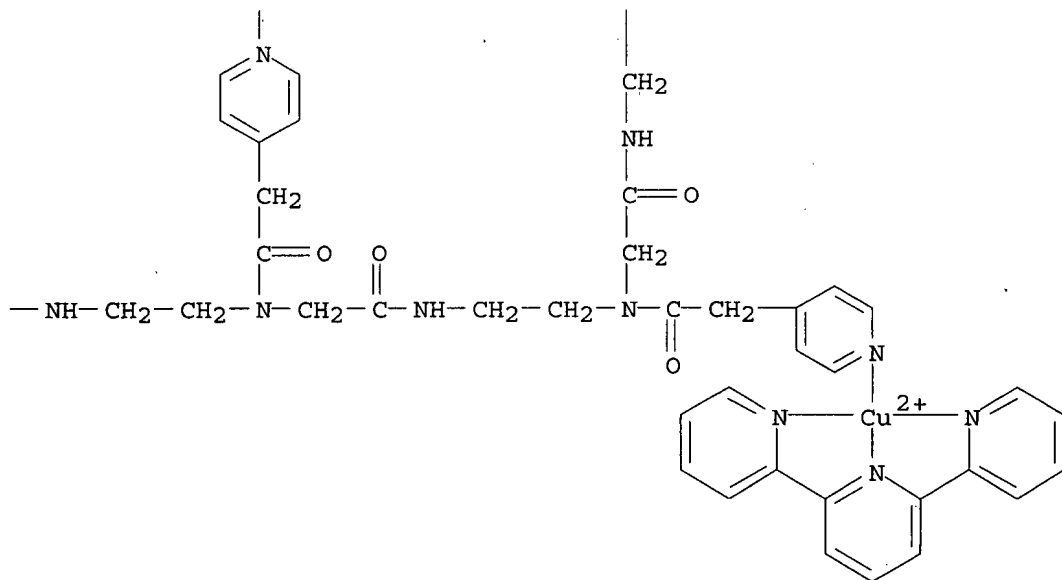
PAGE 1-B

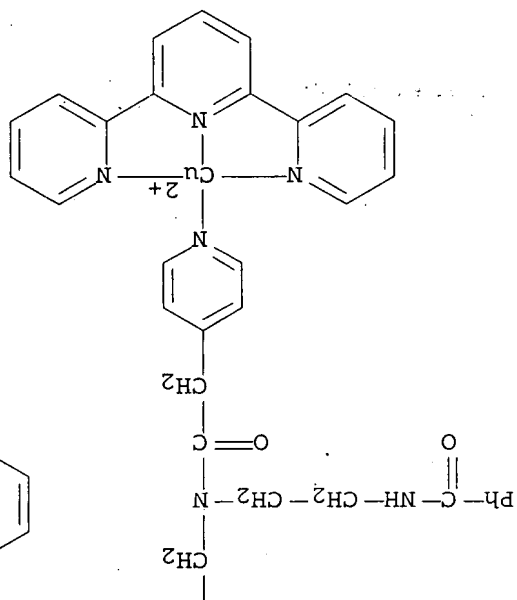
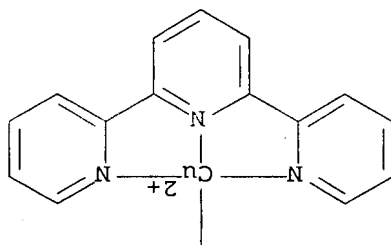


PAGE 2-A

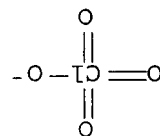


PAGE 2-B





CM 2
CRN 14797-73-0
CMF C1 04



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE IN THE RE FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:438295 HCAPLUS
DOCUMENT NUMBER: 143:358931

TITLE:

Probing the stability and structure of
metalloporphyrin complexes with basic peptides
by mass spectrometry

AUTHOR(S):

Jellen, Emily E.; Ryzhov, Victor
Department of Chemistry and Biochemistry, Northern
Illinois University, DeKalb, IL, 60115, USA
European Journal of Mass Spectrometry (2005), 11(1),
65-72

SOURCE:

CODEN: EJMSEL; ISSN: 1469-0667

PUBLISHER:

IM Publications

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The stability and structure of noncovalent complexes of various
peptides containing basic amino acid residues (Arg, Lys) with
metalloporphyrins were studied in a quadrupole ion trap mass

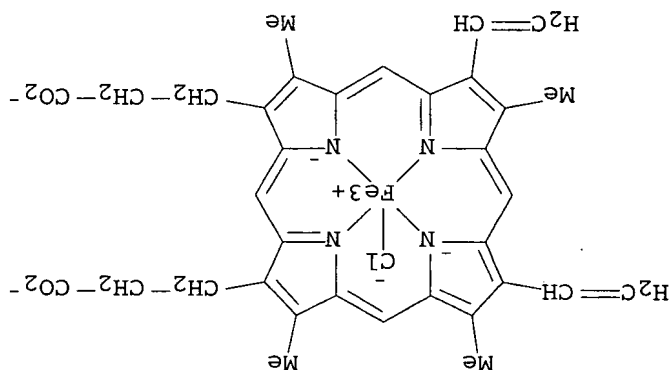
spectrometer. The complexes of heme and three other metalloporphyrins with a variety of basic **peptides** and model systems were formed via electrospray ionization (ESI) and their stability was probed by energy-variable collision-induced dissociation (CID). A linear dependence for basic **peptides** and model compds./metalloporphyrin complexes was observed. This dependence was used to evaluate relative bond strength. These results were then compared with previous data obtained for complexes of metalloporphyrins with His-containing **peptides** and **peptides** containing no basic amino acids. The binding strengths of Lys-containing **peptide** complexes in the gas phase is almost as strong as that of Arg-containing complexes. Both systems showed stronger binding than His-containing **peptides** studied previously. To probe the structure of Arg and Lys noncovalent complexes (charge solvation vs. salt bridges), two techniques, CID and ion-mol. reactions, were used. CID expts. indicate that the gas-phase complexes are most likely formed by charge solvation of the central metal ion in the metalloporphyrin by basic side chains of Arg or Lys. Results from the ion-mol. reaction studies are consistent with the charge solvation structure as well.

- CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 34, 73
- ST metalloporphyrin basic **peptide** formation stability structure
mass spectrometry; charge solvation structure
metalloporphyrin basic **peptide**; zwitterionic structure
metalloporphyrin basic **peptide**
- IT **Peptides**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(basic; stability and structure of metalloporphyrin complexes with
basic **peptides** studied by **mass spectrometry**
)
- IT Molecular structure
(of metalloporphyrin complexes with basic **peptides** studied by
mass spectrometry)
- IT **Transition metal** complexes
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM
(Formation, nonpreparative); RACT (Reactant or reagent)
(porphyrin; stability and structure of metalloporphyrin complexes with
basic **peptides** studied by **mass spectrometry**
)
- IT Collision-induced dissociation
Ion-molecule reaction
Mass spectra
(stability and structure of metalloporphyrin complexes with basic
peptides studied by **mass spectrometry**)
- IT Metalloporphyrins
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM
(Formation, nonpreparative); RACT (Reactant or reagent)
(**transition metal**; stability and structure of
metalloporphyrin complexes with basic **peptides** studied by
mass spectrometry)
- IT 56-87-1D, L-Lysine, metalloporphyrin complexes 74-79-3D, L-Arginine,
metalloporphyrin complexes 107-43-7D, Betaine, metalloporphyrin
complexes 541-15-1D, L-Carnitine, metalloporphyrin complexes
687-64-9D, L-Lysine methyl ester, metalloporphyrin complexes 997-62-6D,
metalloporphyrin complexes 2577-94-8D, metalloporphyrin complexes
6249-56-5D, 3-Carboxypropyltrimethylammonium chloride, metalloporphyrin
complexes 15958-92-6D, 1-8-Bradykinin, metalloporphyrin complexes
16009-13-5D, Hemin chloride, complexes with **peptides** and
analogs 16456-81-8D, complexes with **peptides** and analogs

17043-71-9D, metalloporphyrin complexes 32195-55-4D, complexes with peptides and analogs 49557-75-7D, metalloporphyrin complexes 54944-27-3D, metalloporphyrin complexes 60166-10-1D, complexes with peptides and analogs 66157-45-7D, metalloporphyrin complexes 80755-87-9D, metalloporphyrin complexes 169543-78-6D, metalloporphyrin complexes

IT 16009-13-5D, Hemin chloride, complexes with peptides and analogs
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
 (stability and structure of metalloporphyrin complexes with peptides containing basic amino acid residues (Arg, Lys) studied by mass spectrometry)

CN 16009-13-5 HCAPLUS
 Ferrate(2-), chloro[7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropionato(4-)-κN21,κN22,κN23,κN24]-, dihydrogen, (SP-5-13) - (9CI) (CA INDEX NAME)



● 2 H⁺

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2004:118363 HCAPLUS
 DOCUMENT NUMBER: 140:177881
 TITLE: Novel metal complex, and its use in protein amino acid sequence determination method

INVENTOR(S): Kamiyama, Kenichi; Okamura, Takashi; Norioka, Shigemasa; Nakazawa, Takashi; Kuyama, Hiroki; Ando, Eiji
 PATENT ASSIGNEE(S): Shimizu Corporation, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 29 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004-045292	A1	20040212	JP 2002-204864	20020712
US 2004029181	A1	20040212	US 2003-614324	20030708
PRIORITY APPLN. INFO.:			JP 2002-204864	A 20020712

OTHER SOURCE(S): MARPAT 140:177881

AB A novel metal complex is provided, which is useful as a protein or **peptide** amino acid sequence determination reagent. Also provided is a protein/**peptide** amino acid sequence determination method using the novel metal complex. This metal complex possesses a functional group capable of forming a covalent bond with an amino group of the N-terminal amino acid residue of a protein or **peptide**, or with a carboxyl group of the C-terminal amino acid residue of a protein or **peptide**. Normally, the functional group is contained in a ligand. The method comprises reacting the metal complex with a protein or **peptide** (A) to be analyzed concerning its amino acid sequence, obtaining a metal complex derivative (B) in which a covalent bond is formed between the functional group of the metal complex and the amino group of the N-terminal amino acid residue of the a protein or **peptide**, or the carboxyl group of the C-terminal amino acid residue of the protein or **peptide**, and analyzing the metal complex derivative by a **mass spectrometry** to determine the amino acid sequence of the protein or **peptide**.

IC ICM G01N033-68

ICS C07D213-22; C07D213-53; C07D213-55; C07D249-18; G01N027-62; C07K001-22

CC 9-16 (Biochemical Methods)

ST metal complex protein **peptide** sequence **mass spectrometry**

IT Amino group

Carboxyl group

Coordination number

Functional groups

Mass spectrometry

Protein sequences

(novel metal complex, and use in protein sequence determination method)

IT **Peptides**, biological studies

Proteins

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(novel metal complex, and use in protein sequence determination method)

IT Ligands

Reagents

Transition metals, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(novel metal complex, and use in protein sequence determination method)

IT **657409-70-6P 657409-72-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(novel metal complex, and use in protein sequence determination method)

IT **657409-70-6P 657409-72-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(novel metal complex, and use in protein sequence determination method)

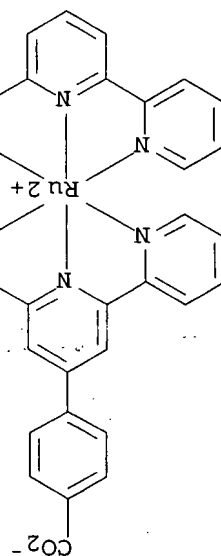
RN **657409-70-6 HCAPLUS**

CN Ruthenium(1+), (2,2':6',2''-terpyridine-κN1,κN1',κN1'') [

4-([2,2':6',2''-terpyridin]-4'-yl)-kN1',kN1''(1:1:2) (9CI) (CA INDEX NAME)
 o]-, (OC-6-23)-, hydrogen hexafluorophosphate(1-)] (1:1:2) (9CI) (CA INDEX

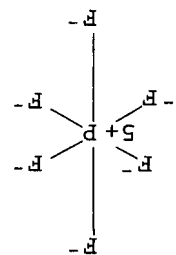
CM 1

CRN 657409-69-3
 CMF C37 H25 N6 O2 Ru
 CCI CCS



CM 2

CRN 16919-18-9
 CMF F6 P
 CCI CCS

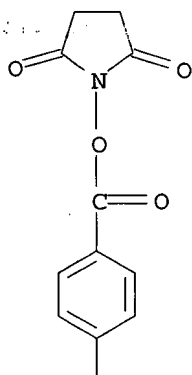


RN 657409-72-8 HCAPLUS
 CN Ruthenium(2+), (2,2':6',2''-terpyridine-kN1',kN1'') [1-[[4-([2,2':6',2''-terpyridin]-4'-yl)-kN1',kN1'')benzoate(1-)] (9CI) (CA INDEX NAME)

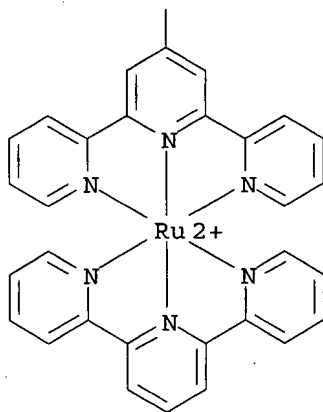
CM 1

CRN 657409-71-7
CMF C41 H29 N7 O4 Ru
CCI CCS

PAGE 1-A

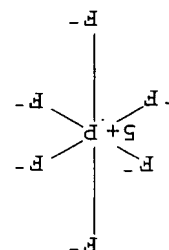


PAGE 2-A



CM 2

CRN 16919-18-9
CMF F6 P



L74 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:901614 HCAPLUS

DOCUMENT NUMBER: 134:202146

TITLE:

Homonuclear PdII and PtII and heteronuclear PdII-AuI and PtII-AuI complexes of a tripod triphosphine ligand: synthesis, characterization and reactions with molecules of biological relevance

AUTHOR(S) :

Sevillano, Paloma; Habtemariam, Abirah; Seijo, M. Ines Garcia; Castineiras, Alfonso; Parsons, Simon; Garcia, M. Esther; Sadler, Peter J.

CORPORATE SOURCE:

Departamento de Química Inorgánica, Universidad de Santiago de Compostela, Facultad de Química, Santiago de Compostela, 15706, Spain

SOURCE:

Australian Journal of Chemistry (2000), 53(8), 635-644
CODEN: AJCHAS; ISSN: 0004-9425

PUBLISHER:

CSIRO Publishing

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S) :

CASREACT 134:202146

AB Complexes Pd(tripod)X₂ [tripod = MeC(CH₂PPH₂)₃; X = Cl (1), Br (2), I (3)] and Pt(tripod)X₂ [X = Cl (4), Br (5), I (6)] were synthesized. In these complexes tripod acts as a bidentate chelating ligand. The uncoordinated P atom can bind to AuI to form the bimetallic complexes PdAu(tripod)X₃ [X = Cl (7), Br (8), I (9)] and PtAu(tripod)X₃ [X = Cl (10), Br (11), I (12)]. Complexes 1-12 were characterized by microanal., FAB mass spectrometry, IR spectroscopy, ³¹P and ¹⁹⁵Pt NMR spectroscopies, and conductivity measurements. The structures of complexes 1-Me₂CO, 4 and 11, as well as that of the unusual complex Cl₂Pt(tripod)AuBr_{0.5}Cl_{0.5} (13), isolated from reaction of Pt(tripod)Br₂ (5), and [Au(thiodiglycol)Cl], were determined. All complexes show square planar geometry for PdII or PtII and linear geometry for AuI. The x-ray crystal structure of 1 showed partial oxidation of the dangling P of the ligand in 50% of the mol. distributed randomly over the lattice. Reactions of complex 4 with the tripeptide glutathione (GSH) showed the formation of [Pt₂(tripod)₂(GS-μ-S)₂]²⁺ (15a). No reaction with N-acetyl-L-methionine (AcMet) or GMP (5'-GMP) was observed. Reactions of [Pt(tripod-O)(ONO₂)₂] (14) with GSH gave [Pt₂(tripod-O)₂(GS-μ-S)₂]²⁺ (15b). Displacement of the S-containing mol. by 5'-GMP in the presence of AuI, via Pt-S bond cleavage, was observed for 15b. PtAu(tripod)Cl₃ 10 reacted with GSH, with initial attack on the AuI center.

CC

78-9 (Inorganic Chemicals and Reactions)

Section cross-reference(s) : 6, 75, 77

ST

crystal structure transition metal

tris(diphenylphosphino)ethane; palladium tris(diphenylphosphino)ethane prepn

structure reaction gold; platinum trisdiphenylphosphinoethane prepn
 reaction gold biomol; phosphinoethane tripodal **transition**
metal homonuclear heteronuclear prepn; gold heteronuclear
 palladium platinum trisdiphenylphosphinoethane prepn; glutathione reaction
 platinum trisdiphenylphosphinoethane; guanosine monophosphate reaction
 platinum trisdiphenylphosphinoethane; acetylmethionine reaction platinum
 trisdiphenylphosphinoethane

IT 327033-73-8 327033-76-1 327033-79-4

327033-79-4D, reaction products with 5'GMP in the presence of gold
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,
 nonpreparative)

(formation and NMR of)

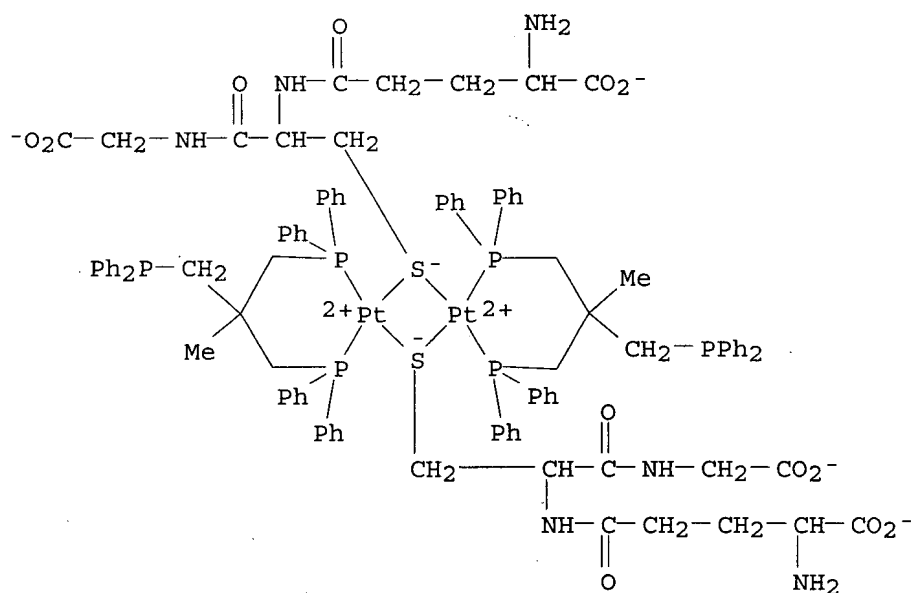
IT 327033-73-8 327033-76-1 327033-79-4

327033-79-4D, reaction products with 5'GMP in the presence of gold
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,
 nonpreparative)

(formation and NMR of)

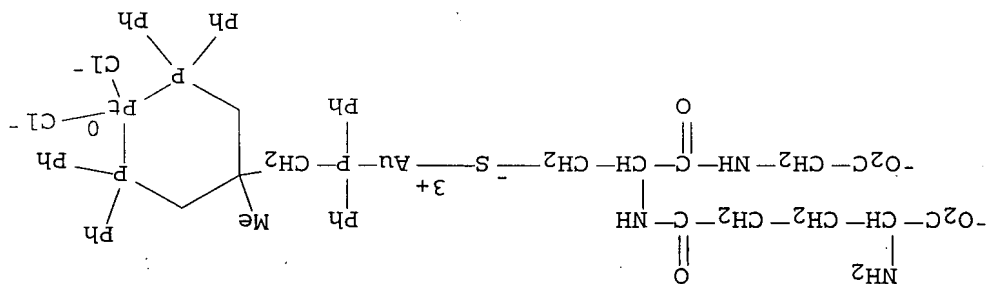
RN 327033-73-8 HCAPLUS

CN Platinate(2-), bis[[2-[(diphenylphosphino)methyl]-2-methyl-1,3-
 propanediyl]]bis[diphenylphosphine-κP]]bis[μ-[L-γ-glutamyl-L-
 cysteinyl-κS:κS-glycinato(3-)]][di- (9CI) (CA INDEX NAME)



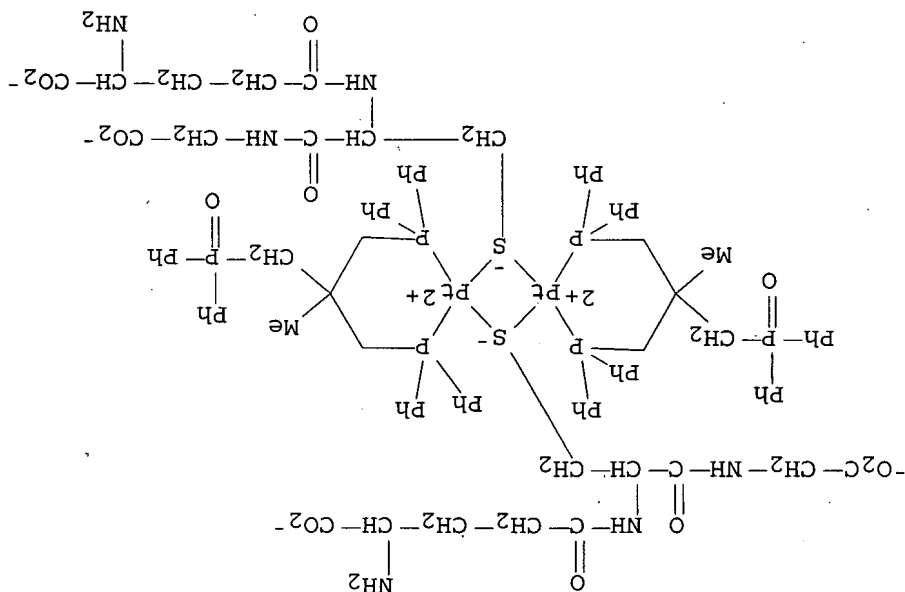
RN 327033-76-1 HCAPLUS

CN Platinate(2-), dichloro[μ-[[2-[(diphenylphosphino-κP)methyl]-2-
 methyl-1,3-propanediyl]]bis[diphenylphosphine-κP]]][[L-γ-
 glutamyl-L-cysteinyl-κS-glycinato(3-)]aurate]-, dihydrogen (9CI)
 (CA INDEX NAME)

● 2 H⁺

RN 327033-79-4 HCAPLUS
 CN Platinate(2-), bis[[3-(diphenylphosphino-kP)-2-[(diphenylphosphino-kP)methyl]-2-methylpropyl]diphenylphosphine oxide]bis[μ-L-γ-glutamyl-L-glycinate(3-)]][di-, tetrahydrogen (9CI)] (CA INDEX NAME)

PAGE 1-A

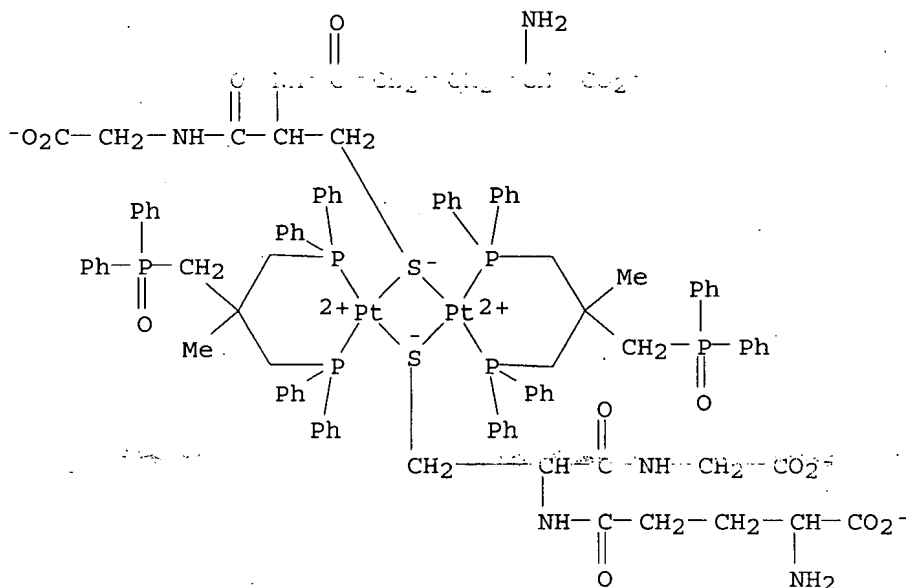


PAGE 2-A

● 4 H⁺

RN 327033-79-4 HCAPLUS
 CN Platinate(2-), bis[[3-(diphenylphosphino-kP)-2-[(diphenylphosphino-kP)methyl]-2-methylpropyl]diphenylphosphine oxide]bis[μ-L-γ-glutamyl-L-glycinate(3-)]][di-, tetrahydrogen (9CI)] (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

● 4 H⁺

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:836623 HCAPLUS

DOCUMENT NUMBER: 134:193701

TITLE: Compositions and conformations of several transition metal complexes with a nonapeptide hormone oxytocin

AUTHOR(S): Wei, Hua; Luo, Xuemei; Wu, Yibing; Yao, Yong; Guo, Zijian; Zhu, Longgen

CORPORATE SOURCE: Coordination Chemistry Institute, State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing, 210093, Peop. Rep. China

SOURCE: Dalton (2000), (22), 4196-4200

CODEN: DALTFG

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Similar co-ordination characteristics of oxytocin (OT) towards CuII, NiII, MnII and ZnII at different pH values have been demonstrated by electrospray mass spectrometry (ESMS) and rationalized by mol. mechanics simulation. At ca. pH 2 oxytocin does not interact with the metal ions; at pH 5 species with metal bound oxytocin were detected, including [OT + H]⁺, [M + OT]²⁺, [M + OT - H]⁺, [M + OT + ClO₄ - + H]²⁺ and [M + OT + ClO₄ -]⁺ and only stable 4N complexes were found at pH ≈ 9. Mol. modeling studies using the Universal force field (UFF) showed that the four N-donor centers of oxytocin prefer the square planar

geometry in complexes of NiII and MnII. For PdII, the Sy(1) coordinated conformer was found to be more stable than the Sy(6) coordinated one. Dramatic conformational changes occur upon oxytocin co-ordinating to NiII, MnII or PdII.

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 2, 78

ST oxytocin complex **transition metal** conformation ESMS
mol mechanics simulation; conformation complex **transition metal** oxytocin mol modeling

IT Conformation

Electrospray ionization **mass spectrometry**

Molecular mechanics

Molecular modeling

Simulation and Modeling, physicochemical

(conformations of **transition metal** complexes with oxytocin)

IT **Transition metal** complexes

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(conformations of **transition metal** complexes with oxytocin)

IT 328123-81-5

RL: PRP (Properties)

(conformations of **transition metal** complexes with oxytocin)

IT 50-56-6DP, Oxytocin, **transition metal** complexes, preparation 50-56-6P, Oxytocin, preparation 7439-96-5DP, Manganese, oxytocin complexes, preparation 7440-02-0DP, Nickel, oxytocin complexes, preparation 7440-50-8DP, Copper, oxytocin complexes, preparation 7440-66-6DP, Zinc, oxytocin complexes, preparation 222716-70-3P
328123-77-9P 328123-78-0P 328123-79-1P
328123-80-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(conformations of **transition metal** complexes with oxytocin)

IT 328123-81-5

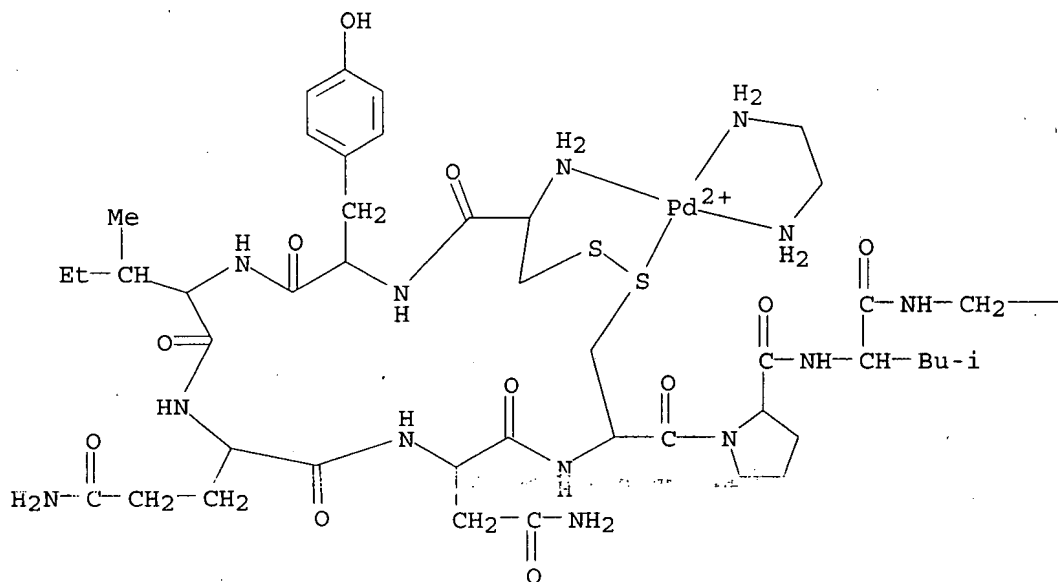
RL: PRP (Properties)

(conformations of **transition metal** complexes with oxytocin)

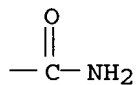
RN 328123-81-5 HCAPLUS

CN Palladium(2+), (oxytocin-κN1,κS)- (9CI) (CA INDEX NAME)

PAGE 1-A

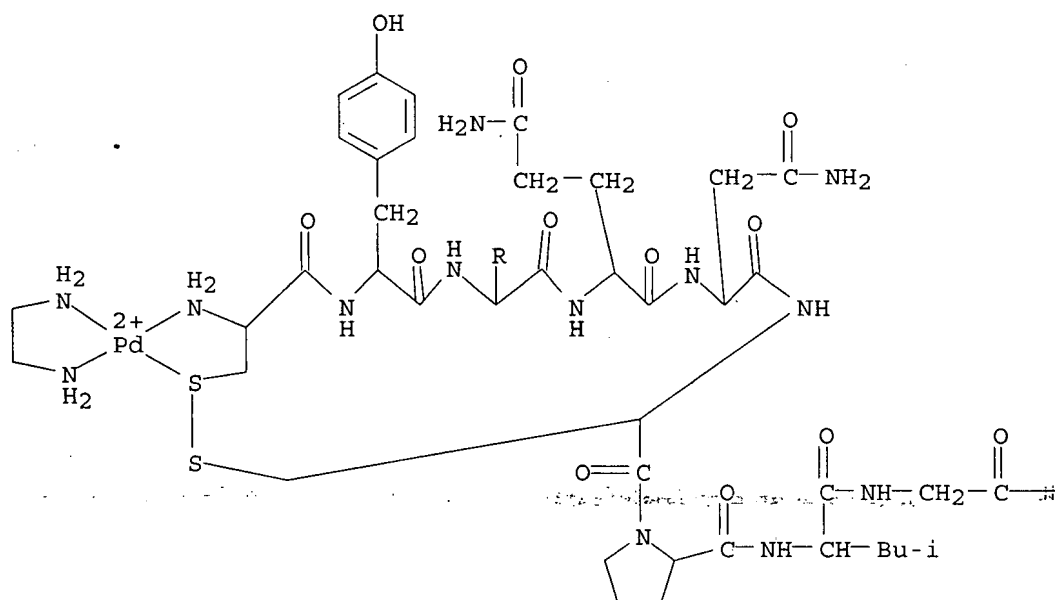


PAGE 1-B



IT 222716-70-3P 328123-77-9P 328123-78-0P
 328123-79-1P 328123-80-4P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (conformations of **transition metal** complexes with
 oxytocin)
 RN 222716-70-3 HCAPLUS
 CN Palladium(2+), (1,2-ethanediamine-κN1,κN2)(oxytocin-
 κN1,κS1)-, (SP-4-3)- (9CI) (CA INDEX NAME)

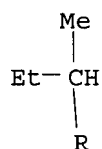
PAGE 1-A



PAGE 1-B

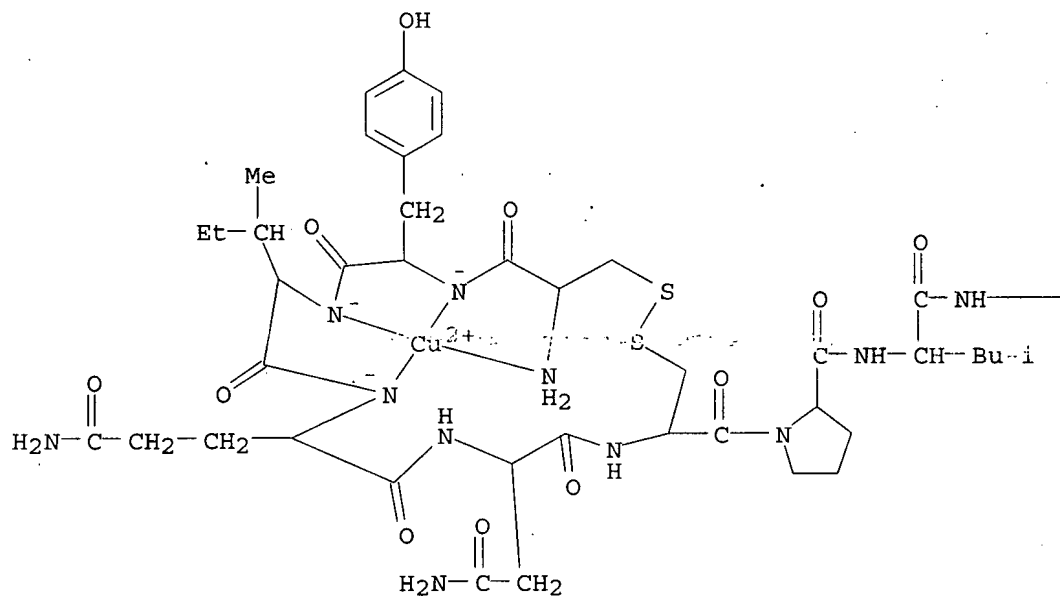
—NH₂

PAGE 2-A

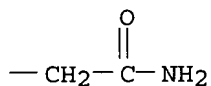


RN 328123-77-9 HCAPLUS
 CN Cuprate(1-), [oxytocinato(4-)-κN1,κN2,κN3,κN4]-
 (9CI) (CA INDEX NAME)

PAGE 1-A

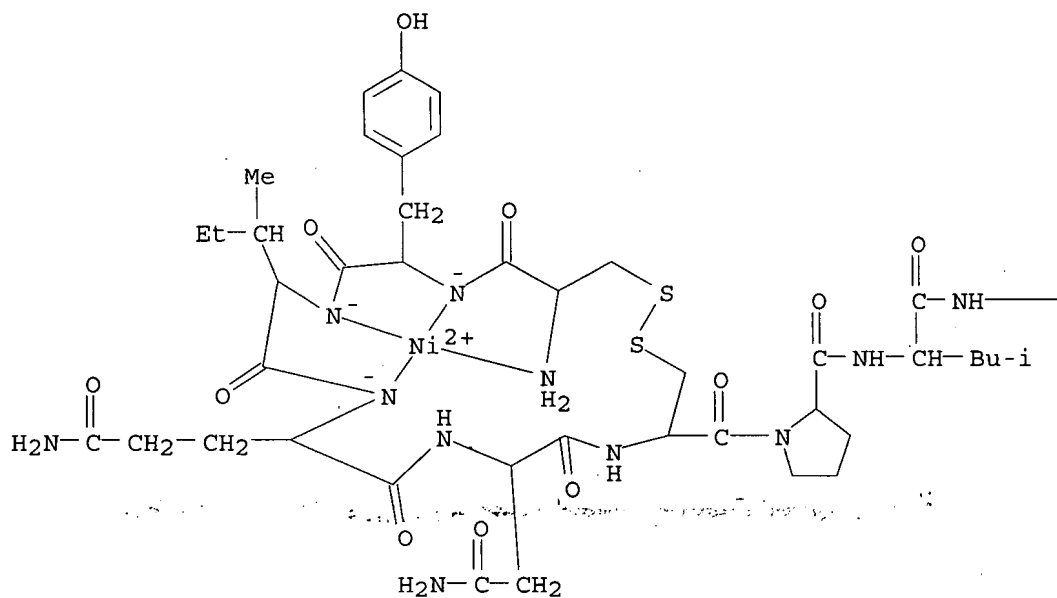


PAGE 1-B

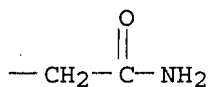


RN 328123-78-0 HCAPLUS
 CN Nickelate(1-), [oxytocinato(4-)-κN1,κN2,κN3,κN4]-,
 (SP-4-2)- (9CI) (CA INDEX NAME)

PAGE 1-A

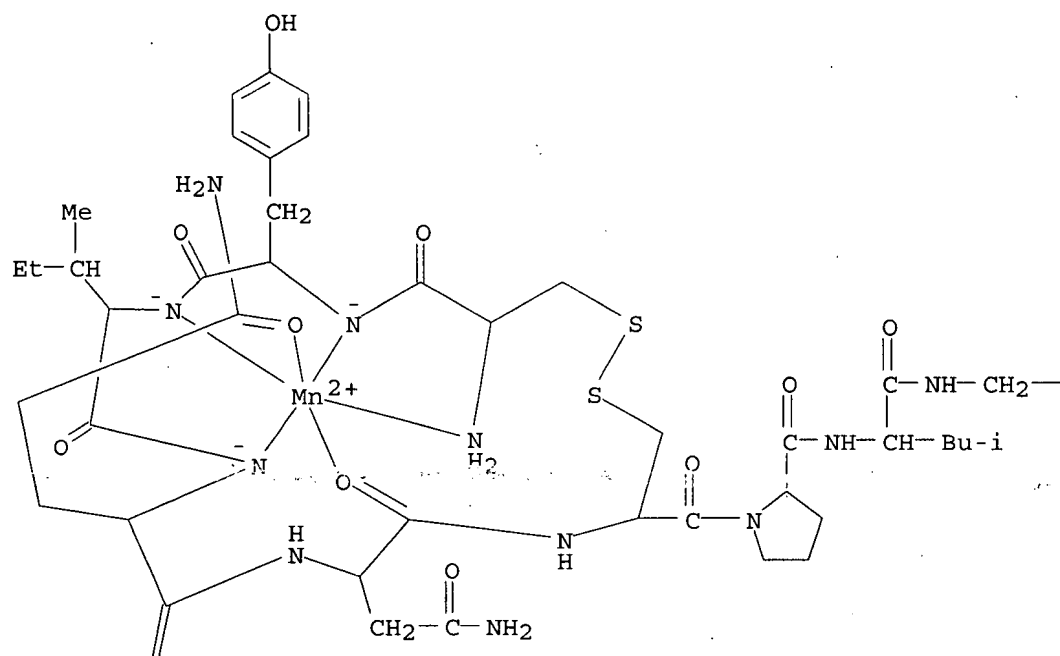


PAGE 1-B

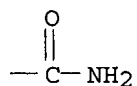


RN 328123-79-1 HCAPLUS
 CN Manganate(1-), [oxytocinato(3-)-κN1,κN2,κN3,κN4,.k
 appa.O4,κO5] - (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



PAGE 2-A

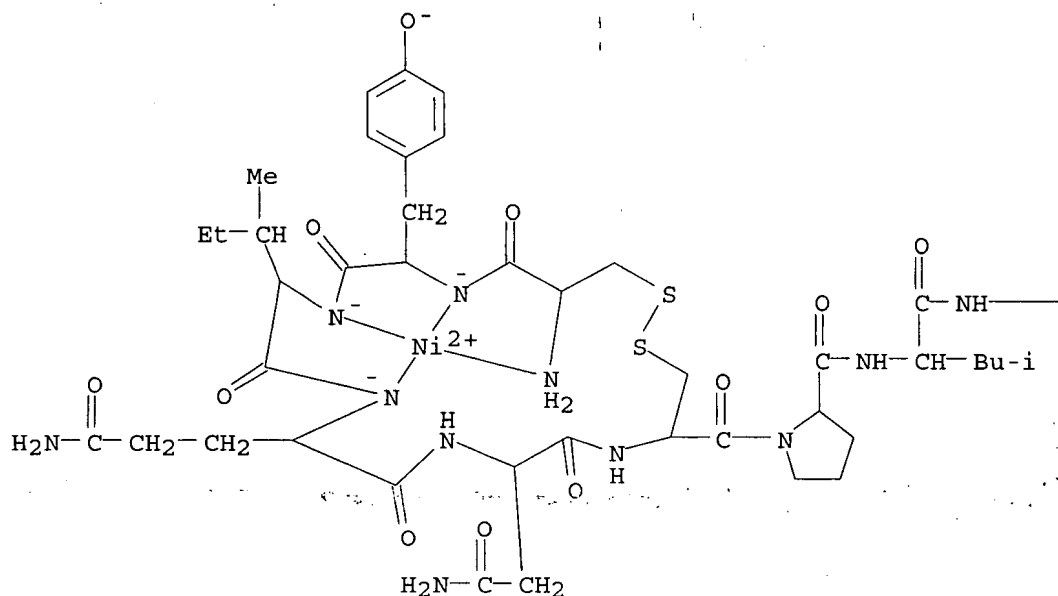


```

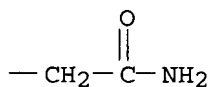
RN      328123-80-4   HCAPLUS
CN      Nickelate(2-), [oxytocinato(4-)-κN1,κN2,κN3,κN4]-,
        (SP-4-2)- (9CI)  (CA INDEX NAME)

```

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:764566 HCAPLUS

DOCUMENT NUMBER: 130:101169

TITLE: A catalytic activity of glass beads, silica gels and anion-exchange resins modified with metal-porphines in oxidative reactions of ascorbic acid

AUTHOR(S): Iwado, Akimasa; Mifune, Masaki; Harada, Harada; Akizawa, Hiromichi; Motohashi, Noriko; Saito, Yutaka

CORPORATE SOURCE: Graduate School of Natural Science and Technology, Okayama University, Okayama, 700-8530, Japan

SOURCE: Inorganica Chimica Acta (1998), 283(1), 44-50

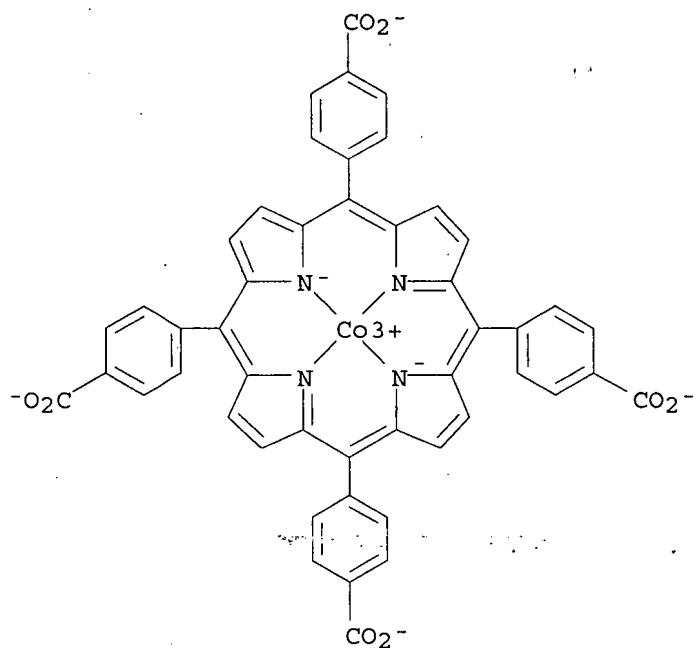
CODEN: ICHAA3; ISSN: 0020-1693

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

- AB An anion-exchange resin was modified with metal-tetrakis(4-sulfophenyl)porphine (M-TSPP) by ion-exchange reaction and phys. adsorption, and silica gels and glass beads were modified by using the acid chloride of metal-tetrakis(4-carboxyphenyl)porphine (M-TCPP) through the **peptide** bond. The supports modified with Co³⁺-porphine accelerate the following redox reaction(s), of which the former is also catalyzed by ascorbate-oxidase (AsA): 2(ascorbate (AsA)+) + O₂ ASO₄ or supports modified with M-porphine → 2(dehydroascorbate (DhAsA)) + 2H₂O; ascorbate (AsA) + O₂ supports modified with M-porphine → dehydroascorbate (DhAsA) + H₂O₂. Formation of DhAsA and H₂O₂ was confirmed by **mass spectrometry** and colored reaction, resp. The supports modified with Co³⁺-porphine would be useful in practice as solid catalysts for the determination of AsA and for the removal of AsA which interferes with the determination of vital materials in clin. assays.
- CC 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms) Section cross-reference(s): 34
- ST oxidn catalyst **transition metal** porphine supported ascorbic acid; glass bead support **transition metal** porphine oxidn catalyst; silica gel support **transition metal** porphine oxidn catalyst; anion exchange reaction support **transition metal** porphine oxidn catalyst
- IT Glass beads
Silica gel, uses
RL: NUU (Other use, unclassified); USES (Uses)
(support for **transition metal** porphines as oxidation catalysts for ascorbic acid)
- IT Oxidation catalysts
(**transition metal** porphines supported on glass beads, silica gels and anion-exchange resins as oxidation catalysts for ascorbic acid)
- IT 9050-97-9, Amberlite IRA 900 53025-53-9, Dowex MSC-1
RL: NUU (Other use, unclassified); USES (Uses)
(support for **transition metal** porphines as oxidation catalysts for ascorbic acid)
- IT 39174-47-5 51329-41-0 60489-11-4 80004-36-0 87261-81-2
88992-32-9 91629-46-8 95763-38-5 129102-32-5 **137090-57-4**
211232-23-4
RL: CAT (Catalyst use); USES (Uses)
(**transition metal** porphines supported on glass beads, silica gels and anion-exchange resins as oxidation catalysts for ascorbic acid)
- IT 50-81-7, Ascorbic acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(**transition metal** porphines supported on glass beads, silica gels and anion-exchange resins as oxidation catalysts for ascorbic acid)
- IT **137090-57-4**
RL: CAT (Catalyst use); USES (Uses)
(**transition metal** porphines supported on glass beads, silica gels and anion-exchange resins as oxidation catalysts for ascorbic acid)
- RN 137090-57-4 HCAPLUS
- CN Cobaltate(3-), [[4,4',4'',4'''-(21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[benzoato]](6-)-κN21,κN22,κN23,κN24]-, (SP-4-1)-(9CI) (CA INDEX NAME)



REFERENCE COUNT:

16

THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT